



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2021 – 01:05 PM EDT

PDB ID : 3KIC  
Title : Crystal structure of adeno-associated virus serotype 3B  
Authors : Lerch, T.F.; Xie, Q.; Chapman, M.S.  
Deposited on : 2009-11-01  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17.1

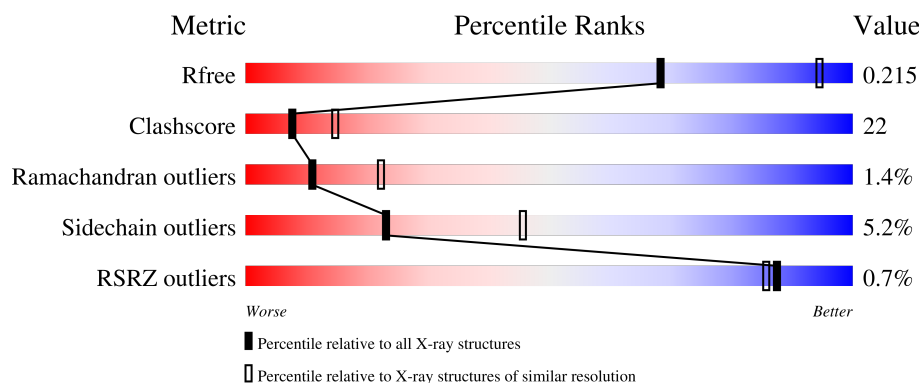
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	<div> <div></div> <div>41%27%•29%</div> </div>
1	B	736	<div> <div>%</div> <div>42%26%•29%</div> </div>
1	C	736	<div> <div>%</div> <div>40%28%•29%</div> </div>
1	D	736	<div> <div>%</div> <div>41%27%•29%</div> </div>
1	E	736	<div> <div>%</div> <div>41%27%•29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	736	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>25%</div> <div>•</div> <div>29%</div> </div> </div>
1	G	736	<div> <div></div> <div>45%</div> <div>24%</div> <div>•</div> <div>29%</div> </div>
1	H	736	<div> <div>%</div> <div> <div></div> <div>42%</div> <div>27%</div> <div>•</div> <div>29%</div> </div> </div>
1	I	736	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>26%</div> <div>•</div> <div>29%</div> </div> </div>
1	J	736	<div> <div></div> <div>42%</div> <div>26%</div> <div>•</div> <div>29%</div> </div>
1	K	736	<div> <div></div> <div>43%</div> <div>26%</div> <div>•</div> <div>29%</div> </div>
1	L	736	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>25%</div> <div>•</div> <div>29%</div> </div> </div>
1	M	736	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>25%</div> <div>•</div> <div>29%</div> </div> </div>
1	N	736	<div> <div></div> <div>44%</div> <div>25%</div> <div>•</div> <div>29%</div> </div>
1	O	736	<div> <div></div> <div>42%</div> <div>26%</div> <div>•</div> <div>29%</div> </div>
1	P	736	<div> <div></div> <div>42%</div> <div>26%</div> <div>•</div> <div>29%</div> </div>
1	Q	736	<div> <div></div> <div>40%</div> <div>28%</div> <div>•</div> <div>29%</div> </div>
1	R	736	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>25%</div> <div>•</div> <div>29%</div> </div> </div>
1	S	736	<div> <div></div> <div>45%</div> <div>24%</div> <div>•</div> <div>29%</div> </div>
1	T	736	<div> <div></div> <div>44%</div> <div>24%</div> <div>•</div> <div>29%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 83520 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

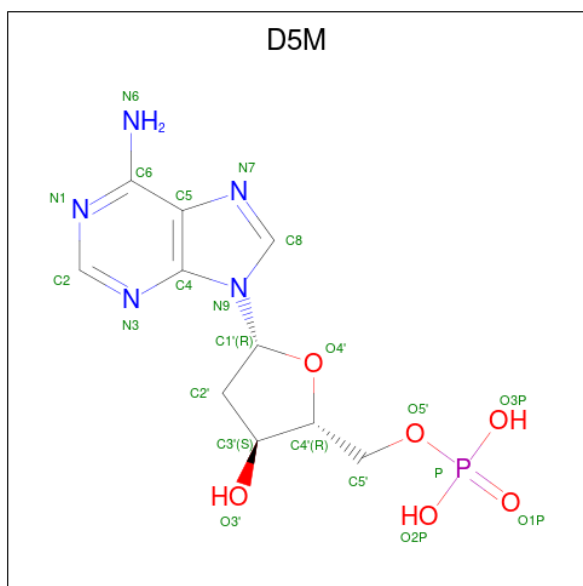
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	B	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	C	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	D	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	E	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	F	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	G	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	H	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	I	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	J	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	K	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	L	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	M	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	N	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	O	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	P	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	R	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	S	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	T	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	G	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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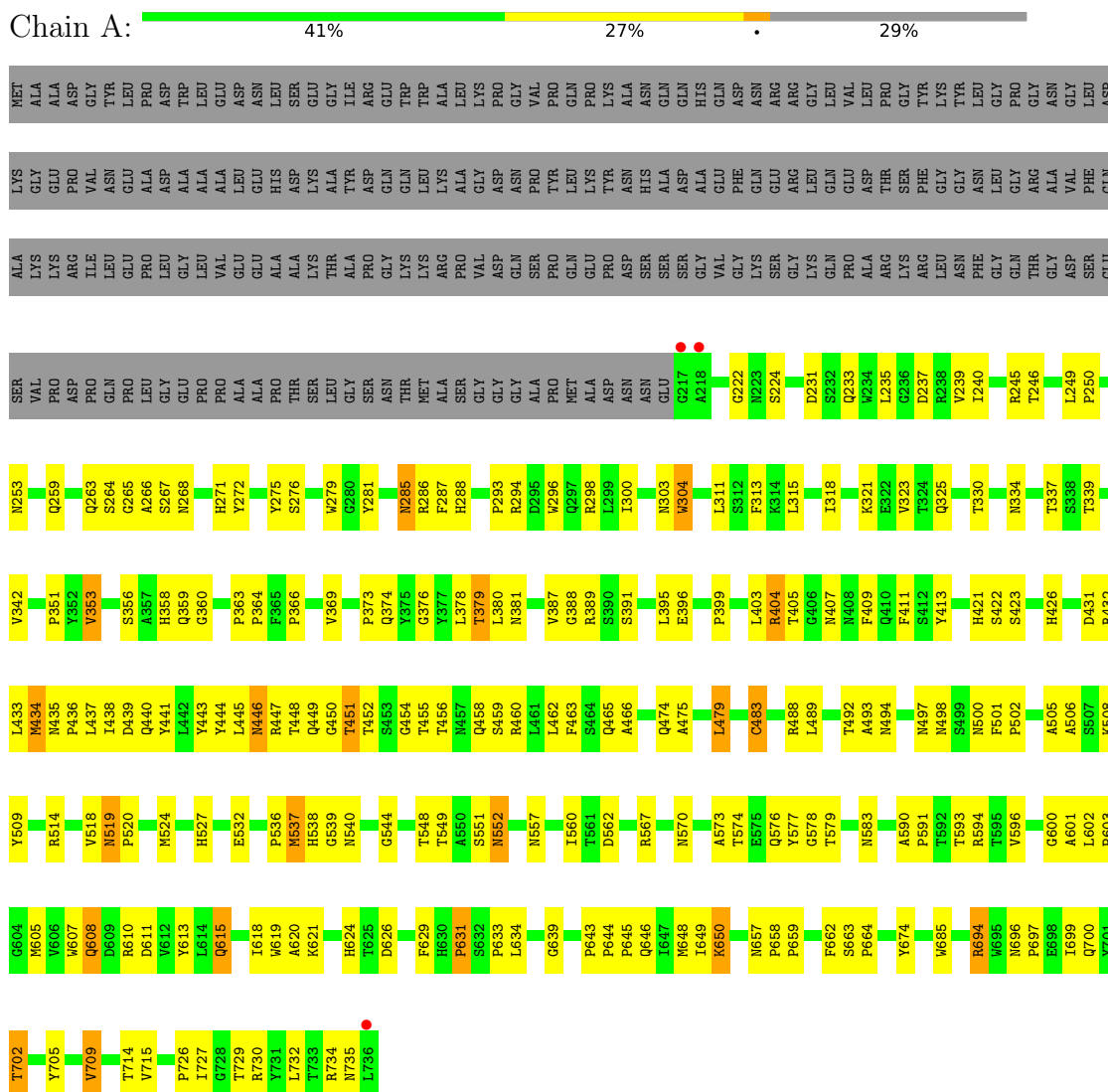
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	I	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	J	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	K	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	L	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	M	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	N	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	O	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	P	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	Q	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	R	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	S	1	Total 22	C 10	N 5	O 6	P 1	0	0
2	T	1	Total 22	C 10	N 5	O 6	P 1	0	0

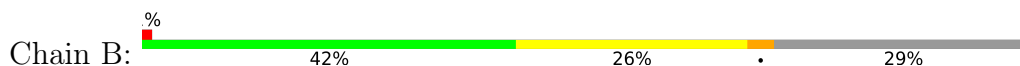
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

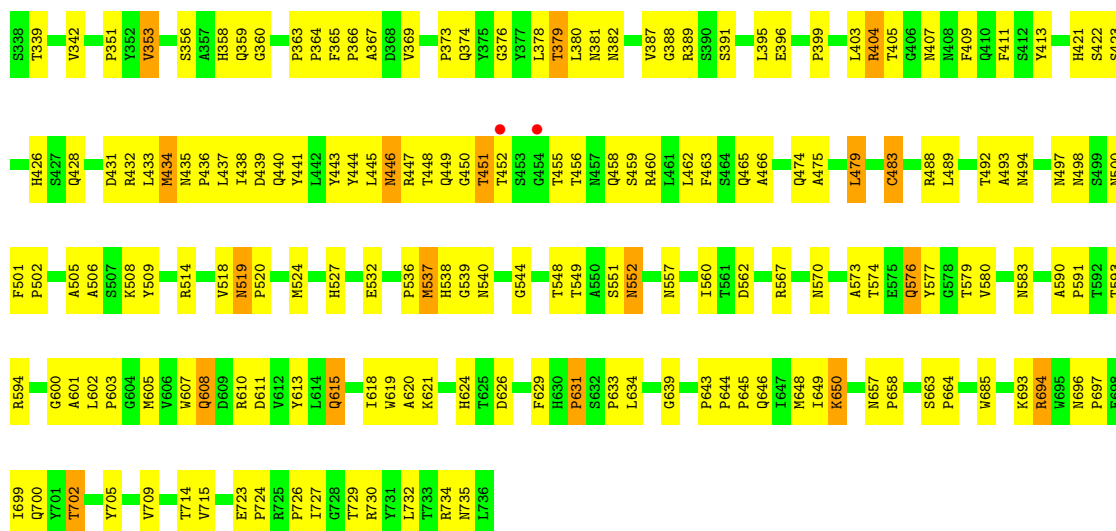
#### • Molecule 1: Capsid protein VP1



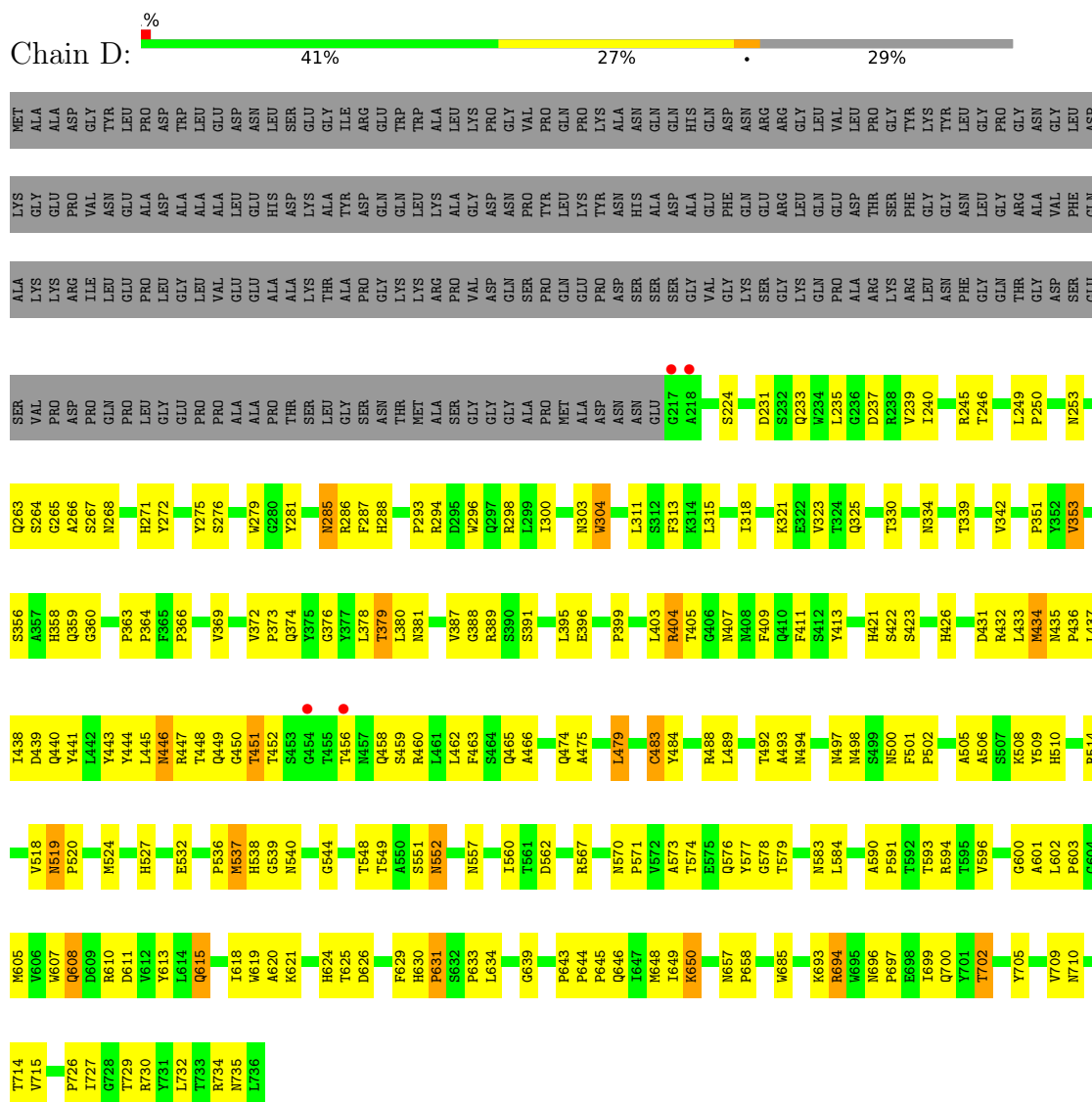
#### • Molecule 1: Capsid protein VP1

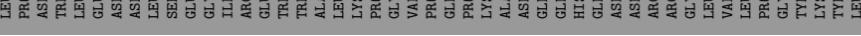




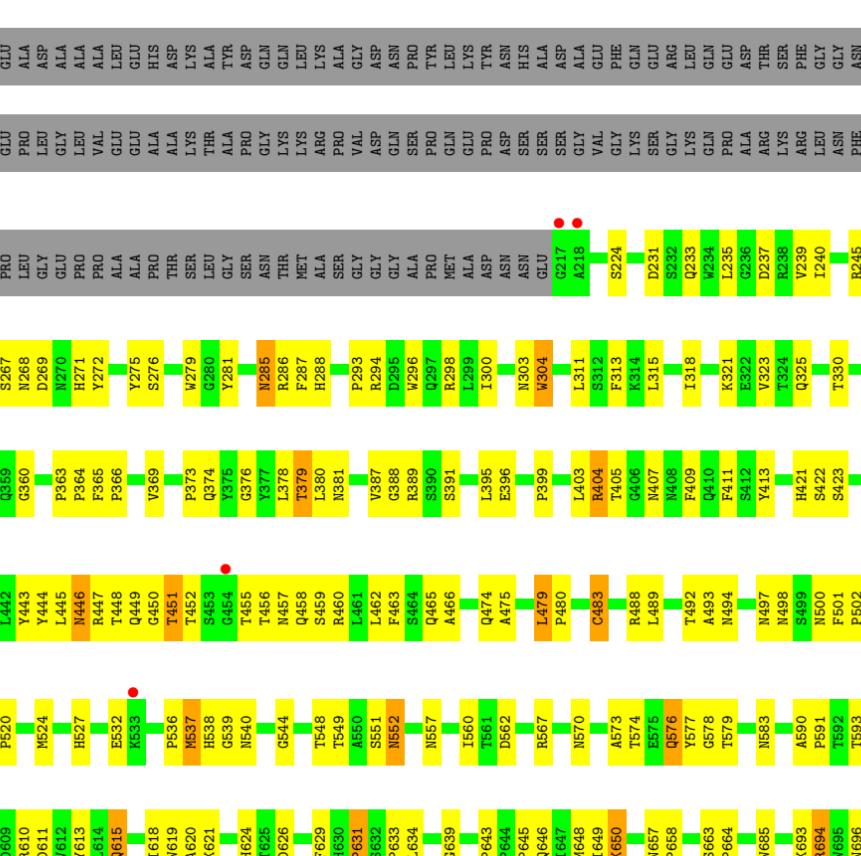


### ● Molecule 1: Capsid protein VP1



Chain E: 

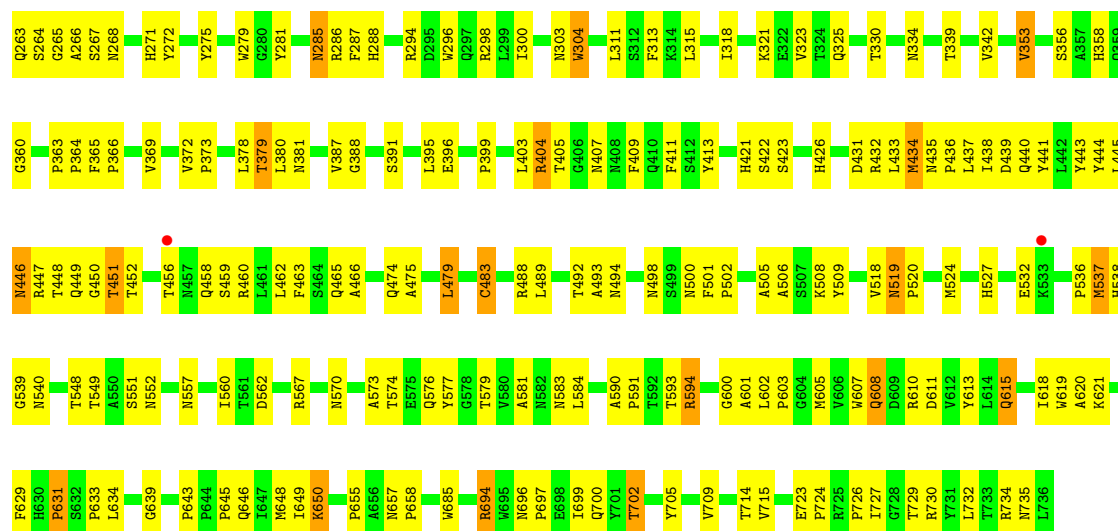
Category	Percentage	Color
Green	41%	Green
Yellow	27%	Yellow
Grey	29%	Grey



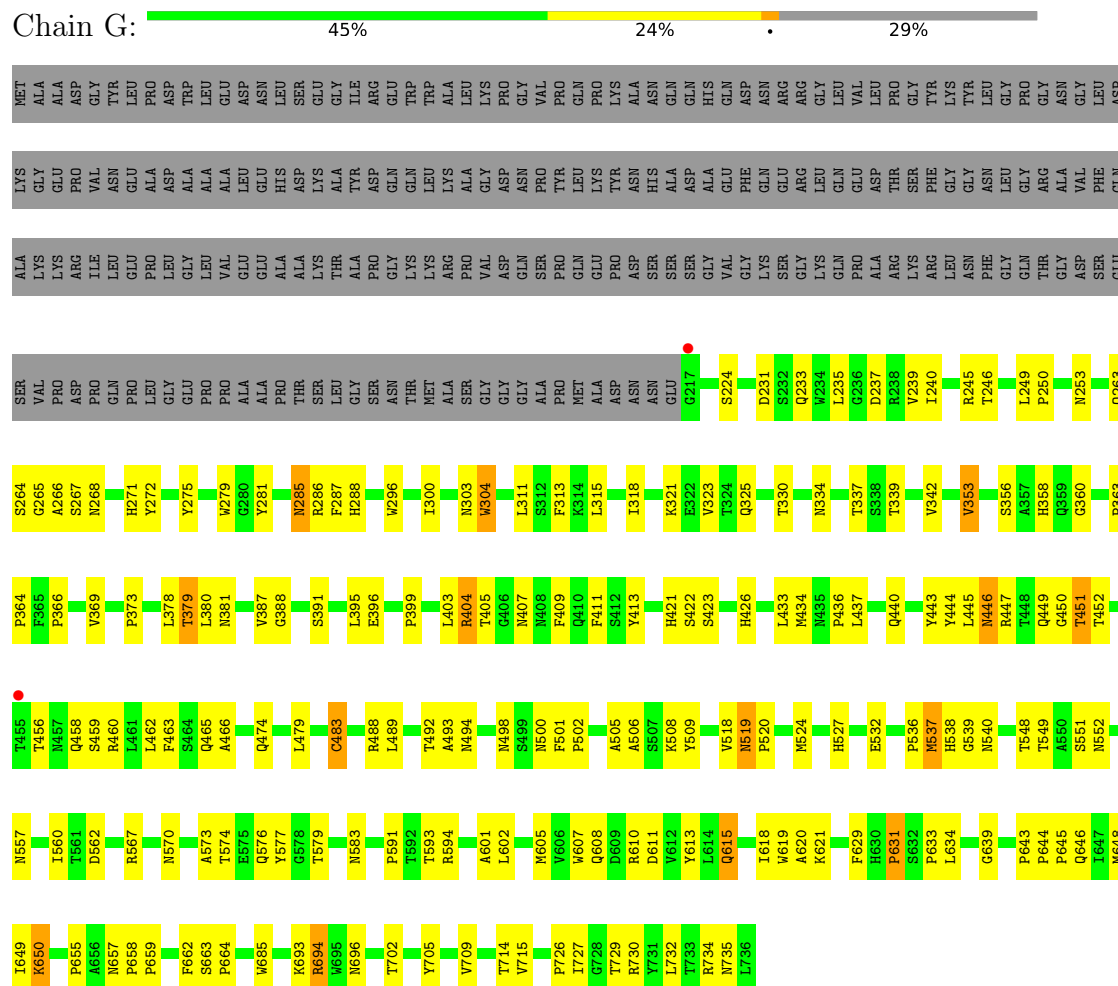
The grid contains 100 colored squares, each with a 3-letter code. The colors correspond to the three categories: Green (41 squares), Yellow (27 squares), and Grey (29 squares). The codes are arranged in a 10x10 grid, with some squares having a red dot in the top right corner.

Chain F: 

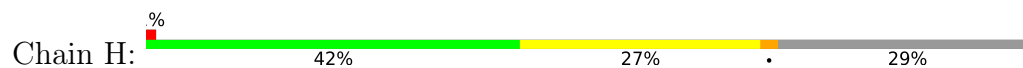
Category	Percentage
Green	43%
Yellow	25%
Grey	29%



### • Molecule 1: Capsid protein VP1



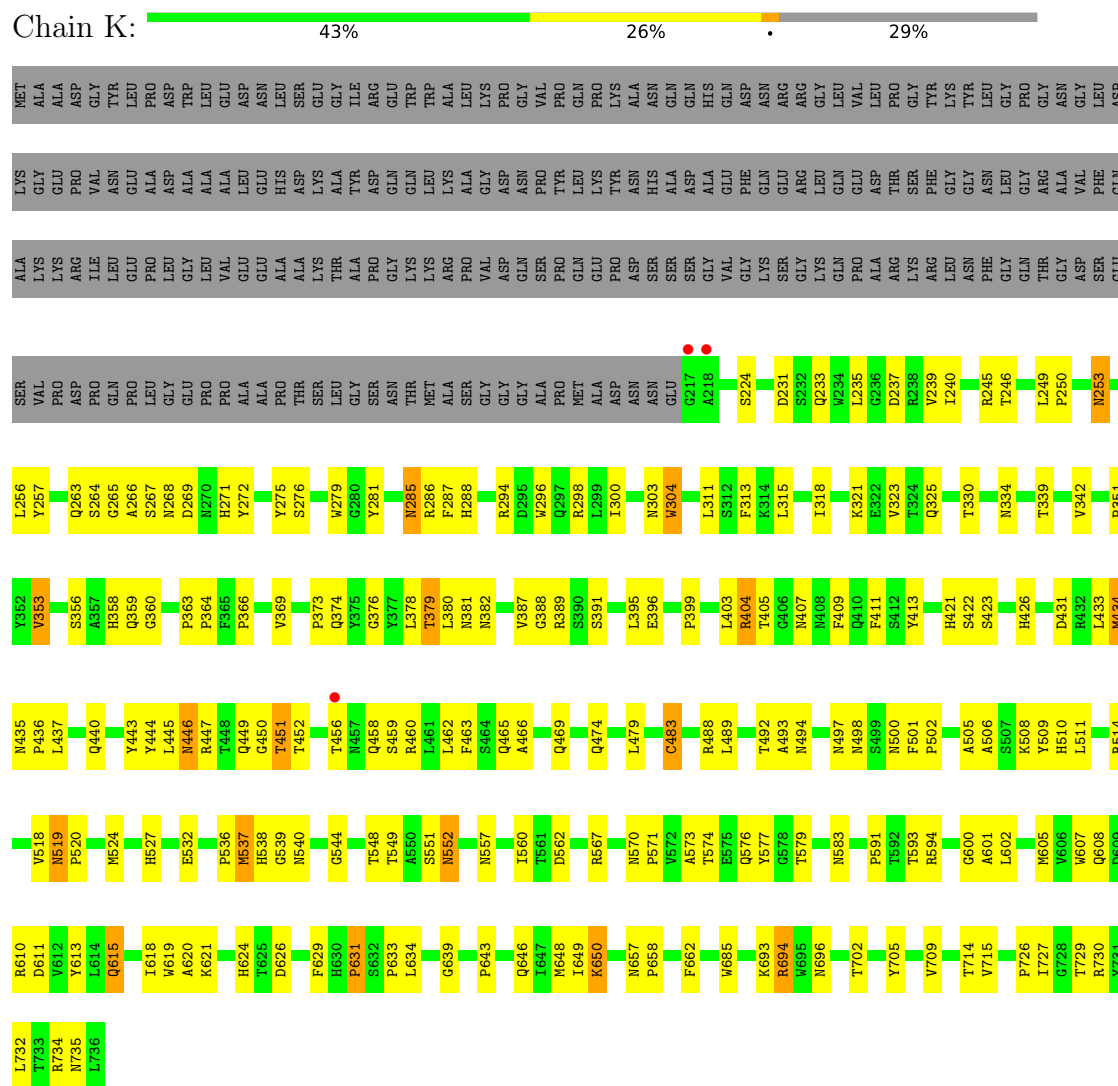
### • Molecule 1: Capsid protein VP1



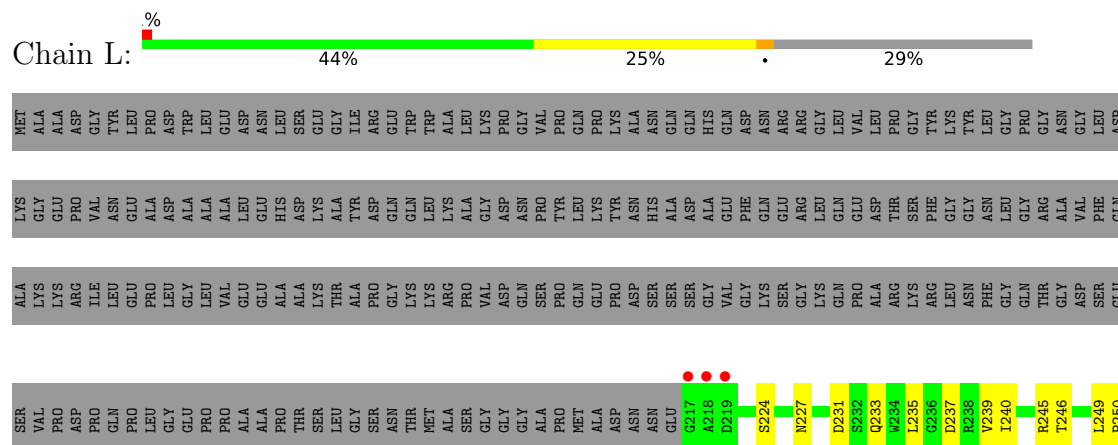




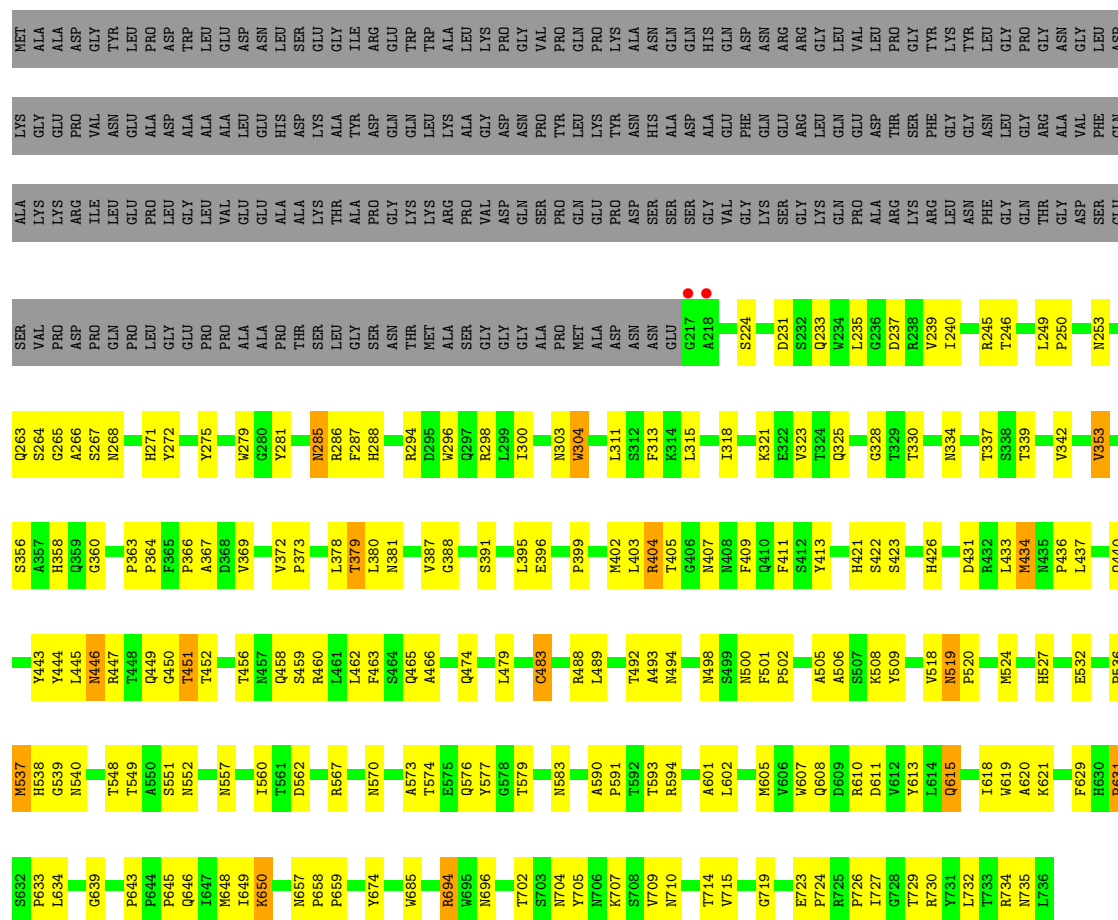
## ● Molecule 1: Capsid protein VP1



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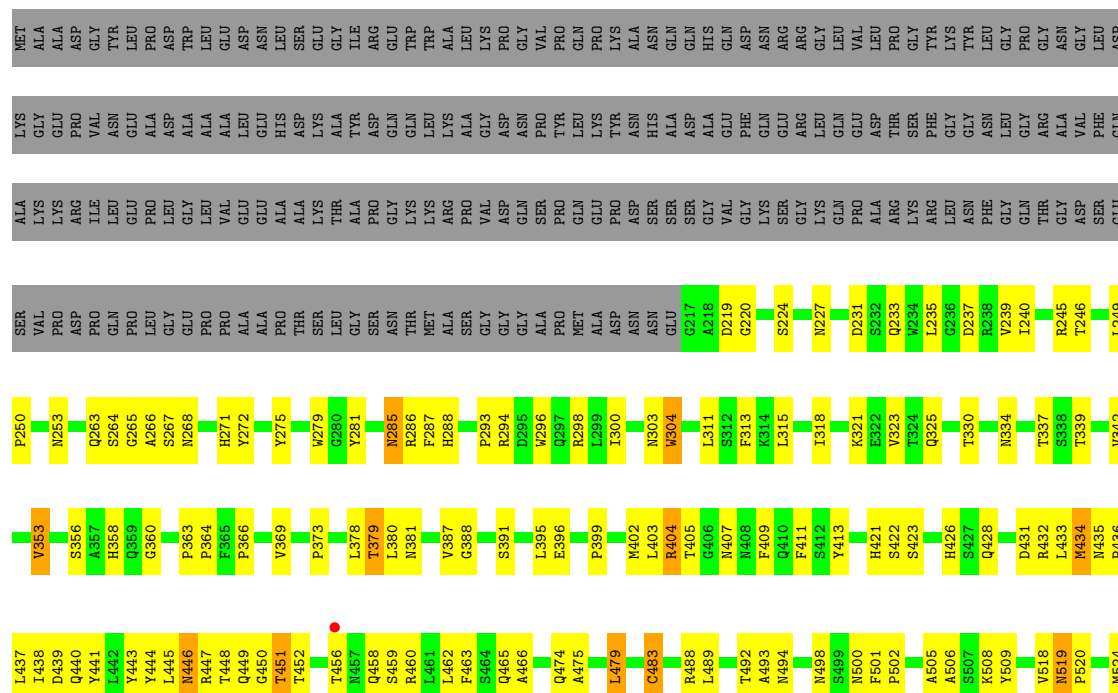


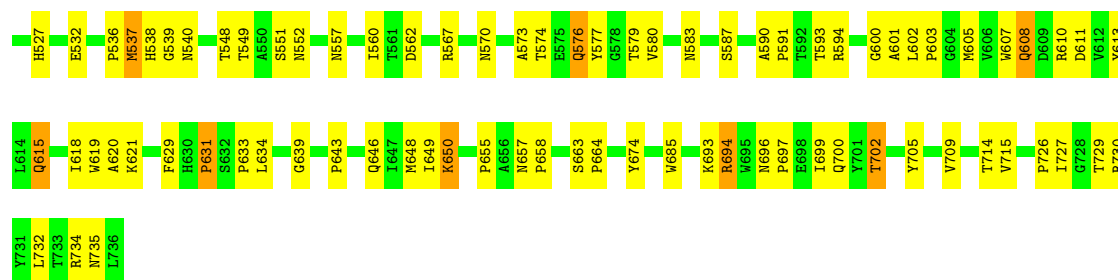




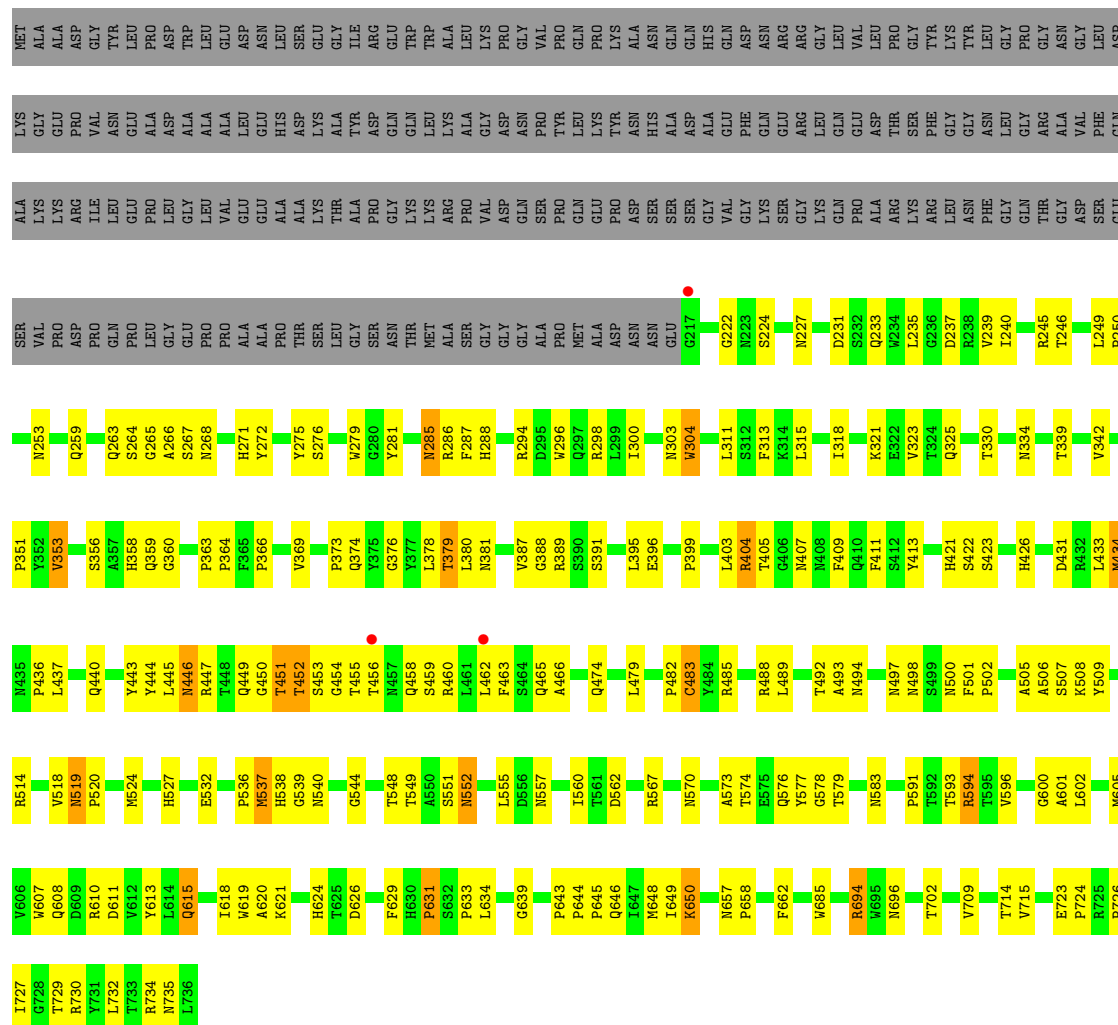
# Molecule 1: Capsid protein VP1

Chain O: 42% 26% 29%

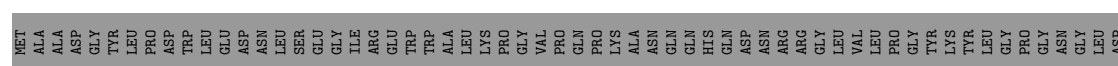


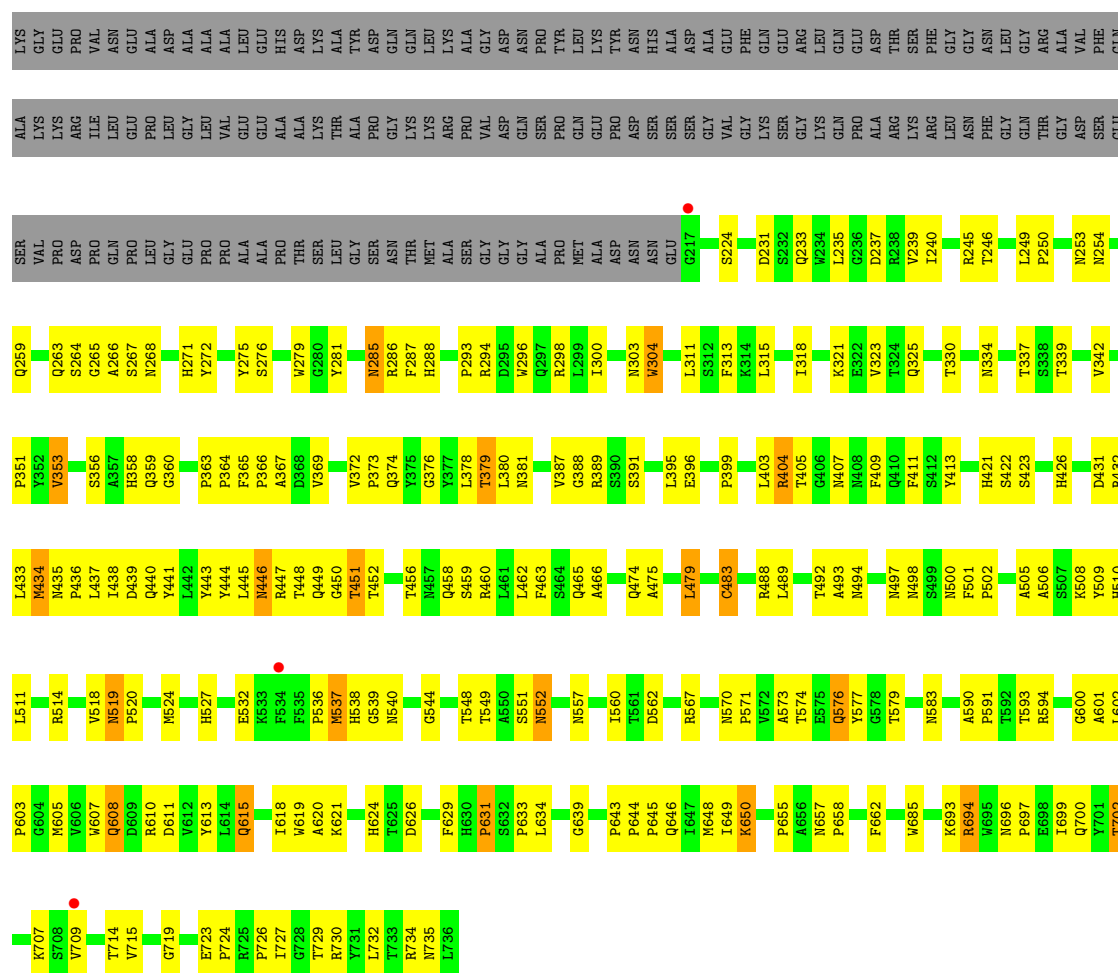


• Molecule 1: Capsid protein VP1

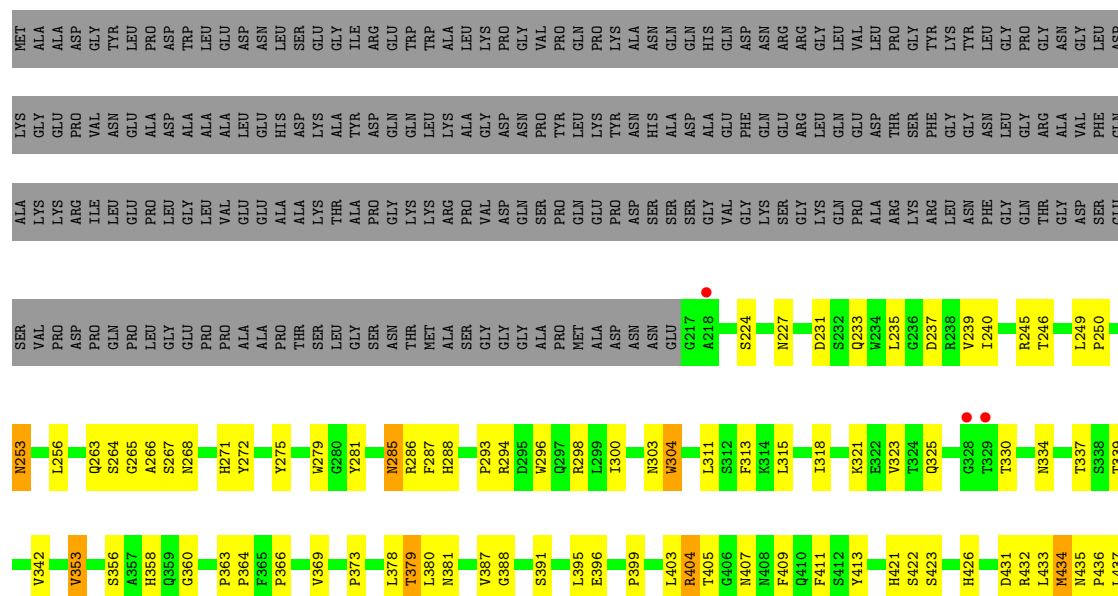


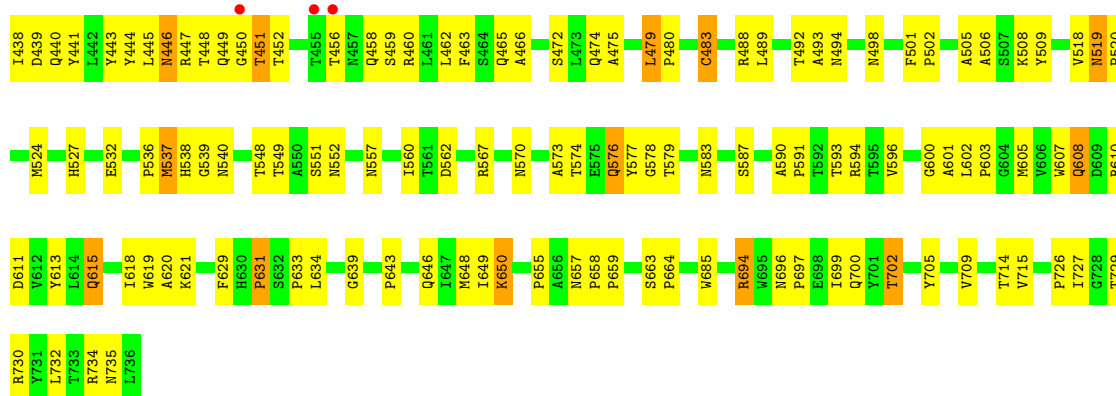
• Molecule 1: Capsid protein VP1



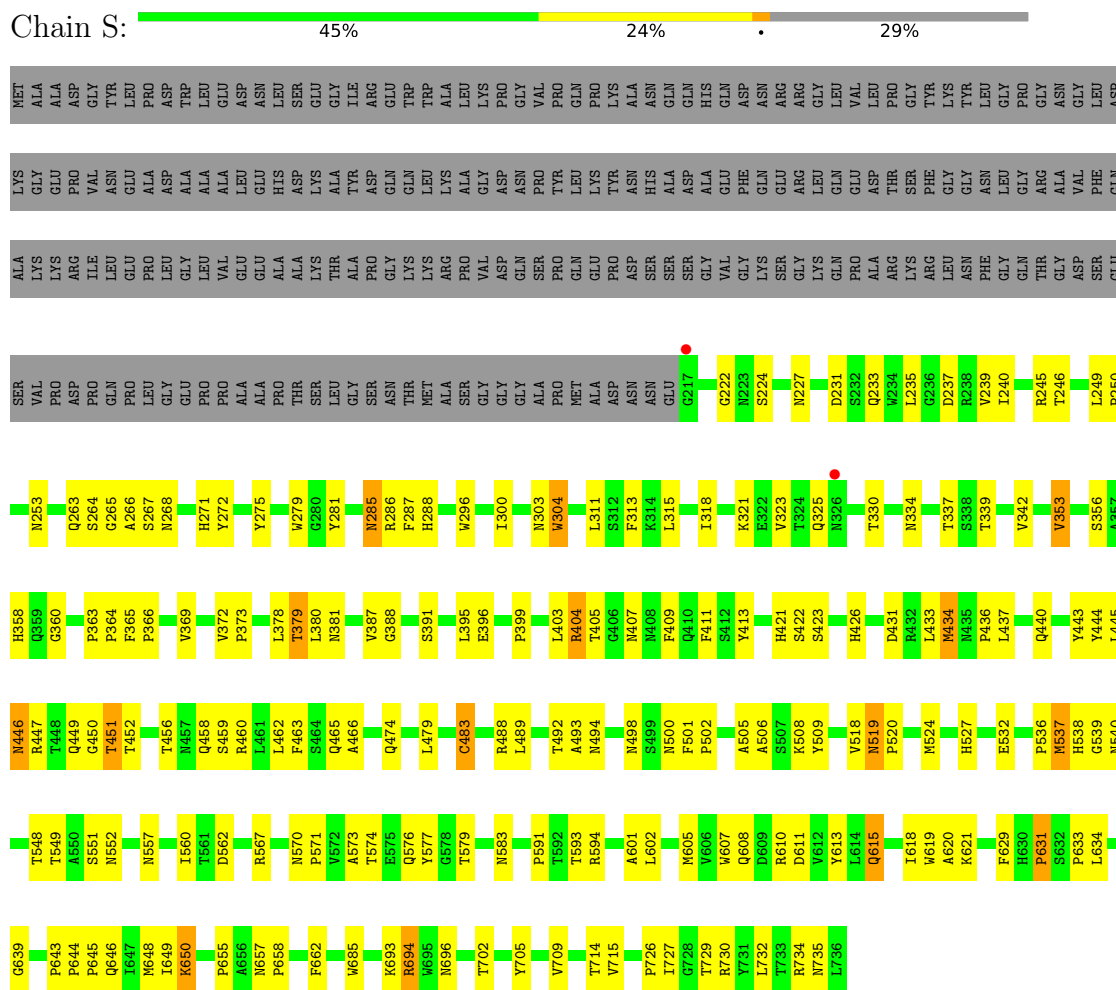


• Molecule 1: Capsid protein VP1

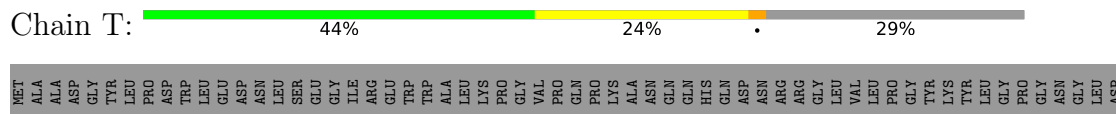




### • Molecule 1: Capsid protein VP1



### • Molecule 1: Capsid protein VP1



H630	P631	S632	P633	L634	G639	P643	Q646	M648	I649	K650	P655	N657	P658	P659	G685	K693	R694	W695	N696	T702	Y705	V709	T714	V715	P726	T727	G728	T729	R730	Y731	L732	T733	R734	N735	L736																																
P536	M537	H538	G539	N540	T543	T549	A550	S551	N552	N557	I560	D562	R567	N570	P571	A573	T574	E575	Q576	Y577	T579	N583	P591	T592	T593	R594	A601	L602	M605	V606	W607	Q608	D609	R610	D611	V612	Y613	L614	Q615	I618	W619	A620	K621	F629																							
Q440	Y443	Y444	L445	M446	R447	T448	Q449	Q450	T451	T452	T456	N457	Q458	S459	R460	L461	L462	F463	S464	Q465	A466	Q474	L479	L479	C483	R488	L489	T492	A493	N494	N498	S499	N500	F501	P502	A505	A506	S507	K508	Y509	V518	N519	P520	M524	L433	M527	E532																				
Y348	V353	S356	A357	H358	G359	G360	P363	P364	F365	P366	V369	P373	L378	T379	L380	N381	V387	G388	S391	L395	E396	P399	L403	R404	T405	G406	N407	N408	F409	Q410	F411	S412	Y413	H421	S422	S423	H426	D431	R432	L433	M434	N435	P436	L437																							
L256	Y257	K258	Q259	Q263	S264	G265	A266	S267	N268	H271	Y272	Y275	W279	Q280	Y281	N285	R286	F287	H288	R294	D295	W296	Q297	R298	L299	I300	N303	W304	L311	S312	F313	R314	L315	I318	K321	E322	V323	T324	Q325	T330	N334	T339	Y342	D345																							
SER	VAL	PRO	ASP	PRO	GLN	PRO	LEU	GLY	PRO	PRO	ALA	ALA	PRO	THR	SER	LEU	GLY	SER	ASN	THR	LYS	MET	ALA	SER	GLY	GLY	GLY	GLN	ASP	ASN	GLU	SER	ASP	ALA	GLY	VAL	GLY	PHE	LYS	SER	GLY	ARG	LYS	GLN	PRO	ALA	ASP	THR	LYS	SER	ARG	ARG	LEU	ASN	GLY	PHE	GLN	GLY	THR	ARG	ALA	ASP	VAL	SER	PHE	GLN	
ALA	LYS	GLU	PRO	ARG	ILE	VAL	LEU	ASN	GLU	ALA	ALA	GLU	GLY	ASP	THR	LYS	ALA	TYR	ASP	GLN	GLY	LYS	LEU	LYS	ARG	PRO	ALA	GLY	VAL	ASP	GLN	ASN	GLY	ASP	ALA	GLY	VAL	GLY	PHE	LYS	SER	GLY	ARG	LYS	GLN	PRO	ALA	ASP	THR	LYS	SER	ARG	ARG	LEU	ASN	GLY	PHE	GLN	GLY	THR	ARG	ALA	ASP	VAL	SER	PHE	GLN

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.70Å 257.70Å 603.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 2.60 48.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	28.1 (14.99-2.60) 28.0 (48.70-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.190 , 0.218 0.190 , 0.215	Depositor DCC
$R_{free}$ test set	3318 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.119 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.125 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.116 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.119 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.119 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.135 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.429 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.475 for h,-h-k,-l	Depositor
Outliers	0 of 128434 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	83520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4282	0.43	0/5843
1	B	0.25	0/4282	0.43	0/5843
1	C	0.25	0/4282	0.43	0/5843
1	D	0.25	0/4282	0.43	0/5843
1	E	0.25	0/4282	0.43	0/5843
1	F	0.25	0/4282	0.43	0/5843
1	G	0.25	0/4282	0.43	0/5843
1	H	0.25	0/4282	0.43	0/5843
1	I	0.25	0/4282	0.43	0/5843
1	J	0.25	0/4282	0.43	0/5843
1	K	0.25	0/4282	0.43	0/5843
1	L	0.25	0/4282	0.43	0/5843
1	M	0.25	0/4282	0.43	0/5843
1	N	0.25	0/4282	0.43	0/5843
1	O	0.25	0/4282	0.43	0/5843
1	P	0.25	0/4282	0.43	0/5843
1	Q	0.25	0/4282	0.43	0/5843
1	R	0.25	0/4282	0.43	0/5843
1	S	0.25	0/4282	0.43	0/5843
1	T	0.25	0/4282	0.43	0/5843
All	All	0.25	0/85640	0.43	0/116860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4154	0	3899	243	8
1	B	4154	0	3899	214	4
1	C	4154	0	3899	247	19
1	D	4154	0	3899	244	0
1	E	4154	0	3899	243	4
1	F	4154	0	3899	211	0
1	G	4154	0	3899	163	3
1	H	4154	0	3899	208	0
1	I	4154	0	3899	238	0
1	J	4154	0	3899	212	0
1	K	4154	0	3899	201	1
1	L	4154	0	3899	172	25
1	M	4154	0	3899	173	0
1	N	4154	0	3899	171	7
1	O	4154	0	3899	215	0
1	P	4154	0	3899	208	9
1	Q	4154	0	3899	247	2
1	R	4154	0	3899	209	0
1	S	4154	0	3899	168	0
1	T	4154	0	3899	168	0
2	A	22	0	12	1	0
2	B	22	0	12	2	0
2	C	22	0	12	2	0
2	D	22	0	12	2	0
2	E	22	0	12	2	0
2	F	22	0	12	2	0
2	G	22	0	12	2	0
2	H	22	0	12	2	0
2	I	22	0	12	1	0
2	J	22	0	12	1	0
2	K	22	0	12	2	0
2	L	22	0	12	2	0
2	M	22	0	12	2	0
2	N	22	0	12	2	0
2	O	22	0	12	2	0
2	P	22	0	12	1	0
2	Q	22	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	22	0	12	1	0
2	S	22	0	12	1	0
2	T	22	0	12	2	0
All	All	83520	0	78220	3544	41

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 3544 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASN:HB3	1:C:520:PRO:HD3	1.46	0.98
1:S:519:ASN:HB3	1:S:520:PRO:HD3	1.46	0.98
1:P:519:ASN:HB3	1:P:520:PRO:HD3	1.45	0.98
1:G:519:ASN:HB3	1:G:520:PRO:HD3	1.45	0.98
1:F:519:ASN:HB3	1:F:520:PRO:HD3	1.45	0.97

The worst 5 of 41 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:THR:OG1	1:K:469:GLN:O[3_445]	1.58	0.62
1:C:267:SER:C	1:L:455:THR:CG2[4_445]	1.59	0.61
1:C:267:SER:O	1:L:456:THR:OG1[4_445]	1.62	0.58
1:C:267:SER:CA	1:L:455:THR:O[4_445]	1.65	0.55
1:C:268:ASN:N	1:L:456:THR:N[4_445]	1.66	0.54

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	11	22
1	B	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	C	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	D	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	11	22
1	E	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	F	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	11	22
1	G	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	H	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	11	22
1	I	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	J	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	K	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	L	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	M	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	N	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	O	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	P	518/736 (70%)	466 (90%)	44 (8%)	8 (2%)	10	21
1	Q	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	11	22
1	R	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	S	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	11	22
1	T	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	11	22
All	All	10360/14720 (70%)	9320 (90%)	899 (9%)	141 (1%)	11	22

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	B	264	SER
1	C	264	SER
1	D	264	SER
1	E	264	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	B	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	C	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	D	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	E	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	F	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	G	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	H	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	I	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	J	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	K	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	L	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	M	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	N	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	O	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	P	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	Q	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	R	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	S	459/627 (73%)	435 (95%)	24 (5%)	23	46
1	T	459/627 (73%)	435 (95%)	24 (5%)	23	46
All	All	9180/12540 (73%)	8700 (95%)	480 (5%)	23	46

5 of 480 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	494	ASN
1	S	451	THR
1	L	694	ARG
1	S	379	THR
1	T	576	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 481 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	374	GLN
1	S	358	HIS
1	L	498	ASN
1	S	253	ASN
1	T	527	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	D5M	K	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	N	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	3 (12%)
2	D5M	O	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	3 (12%)
2	D5M	S	999	-	22,24,24	0.90	1 (4%)	24,36,36	1.31	3 (12%)
2	D5M	P	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	D	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	B	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	2 (8%)
2	D5M	Q	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	D5M	F	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	L	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	3 (12%)
2	D5M	I	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	R	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	G	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	E	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.30	2 (8%)
2	D5M	C	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	3 (12%)
2	D5M	J	999	-	22,24,24	0.92	1 (4%)	24,36,36	1.30	3 (12%)
2	D5M	A	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	3 (12%)
2	D5M	T	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	3 (12%)
2	D5M	H	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.30	3 (12%)
2	D5M	M	999	-	22,24,24	0.91	1 (4%)	24,36,36	1.31	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	K	999	-	-	0/6/22/22	0/3/3/3
2	D5M	N	999	-	-	0/6/22/22	0/3/3/3
2	D5M	O	999	-	-	0/6/22/22	0/3/3/3
2	D5M	S	999	-	-	0/6/22/22	0/3/3/3
2	D5M	P	999	-	-	0/6/22/22	0/3/3/3
2	D5M	D	999	-	-	0/6/22/22	0/3/3/3
2	D5M	B	999	-	-	0/6/22/22	0/3/3/3
2	D5M	Q	999	-	-	0/6/22/22	0/3/3/3
2	D5M	F	999	-	-	0/6/22/22	0/3/3/3
2	D5M	L	999	-	-	0/6/22/22	0/3/3/3
2	D5M	I	999	-	-	0/6/22/22	0/3/3/3
2	D5M	R	999	-	-	0/6/22/22	0/3/3/3
2	D5M	G	999	-	-	0/6/22/22	0/3/3/3
2	D5M	E	999	-	-	0/6/22/22	0/3/3/3
2	D5M	C	999	-	-	0/6/22/22	0/3/3/3
2	D5M	J	999	-	-	0/6/22/22	0/3/3/3
2	D5M	A	999	-	-	0/6/22/22	0/3/3/3
2	D5M	T	999	-	-	0/6/22/22	0/3/3/3
2	D5M	H	999	-	-	0/6/22/22	0/3/3/3
2	D5M	M	999	-	-	0/6/22/22	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	999	D5M	C5-C4	2.65	1.47	1.40
2	J	999	D5M	C5-C4	2.64	1.47	1.40
2	A	999	D5M	C5-C4	2.64	1.47	1.40
2	G	999	D5M	C5-C4	2.64	1.47	1.40
2	R	999	D5M	C5-C4	2.63	1.47	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	999	D5M	N3-C2-N1	-3.28	123.55	128.68
2	A	999	D5M	N3-C2-N1	-3.28	123.55	128.68
2	O	999	D5M	N3-C2-N1	-3.28	123.55	128.68
2	N	999	D5M	N3-C2-N1	-3.28	123.56	128.68
2	L	999	D5M	N3-C2-N1	-3.28	123.56	128.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 33 short contacts:

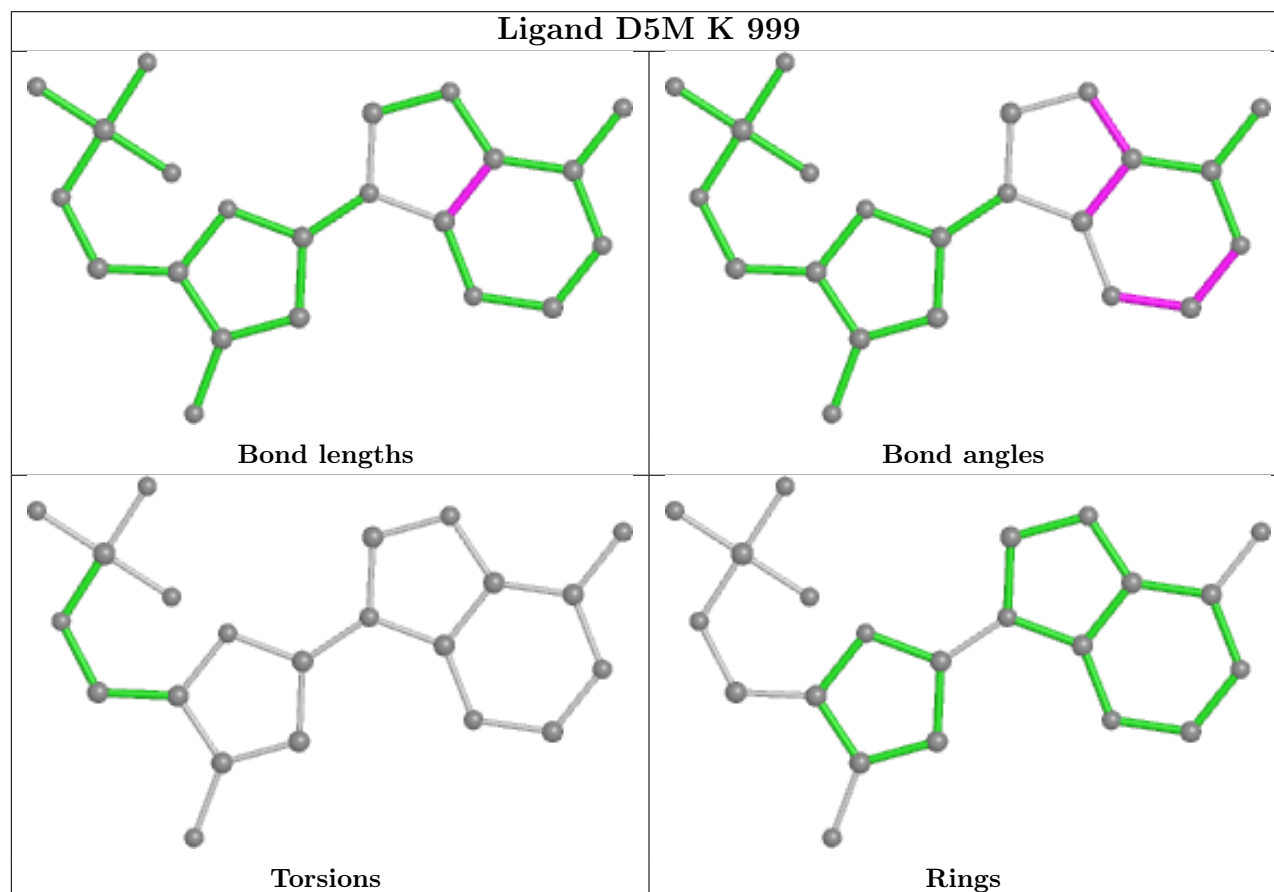
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	999	D5M	2	0
2	N	999	D5M	2	0
2	O	999	D5M	2	0
2	S	999	D5M	1	0
2	P	999	D5M	1	0
2	D	999	D5M	2	0
2	B	999	D5M	2	0
2	Q	999	D5M	1	0
2	F	999	D5M	2	0
2	L	999	D5M	2	0
2	I	999	D5M	1	0
2	R	999	D5M	1	0
2	G	999	D5M	2	0
2	E	999	D5M	2	0
2	C	999	D5M	2	0
2	J	999	D5M	1	0
2	A	999	D5M	1	0
2	T	999	D5M	2	0
2	H	999	D5M	2	0

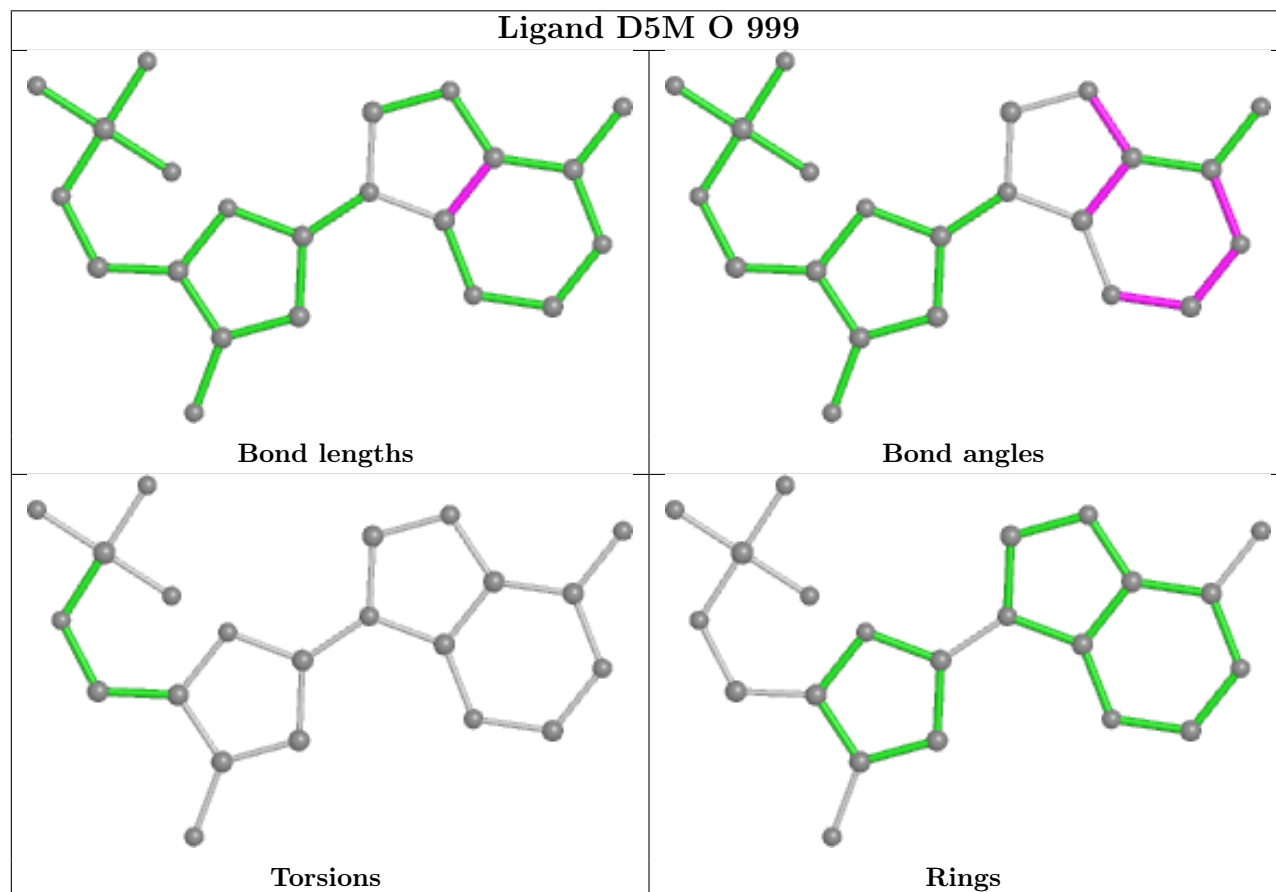
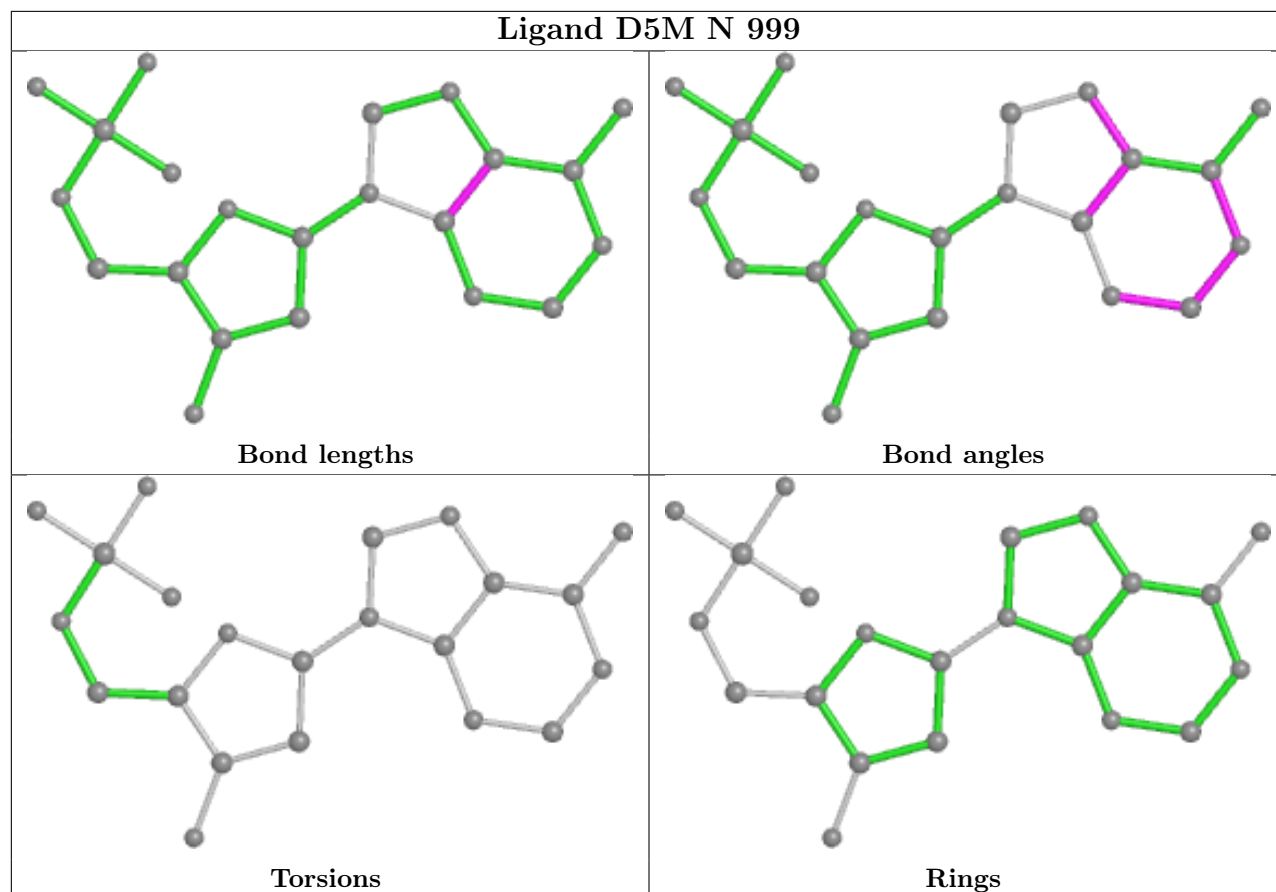
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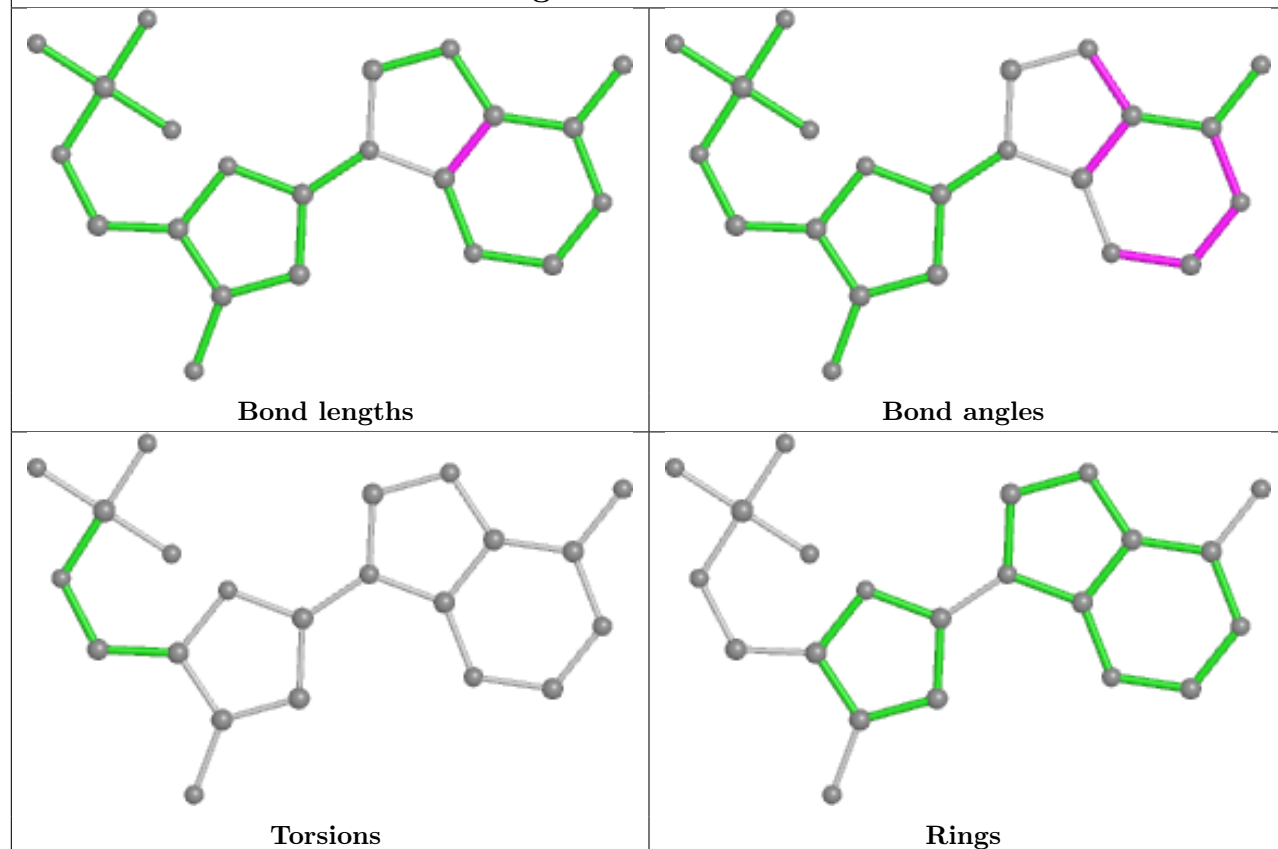
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	999	D5M	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

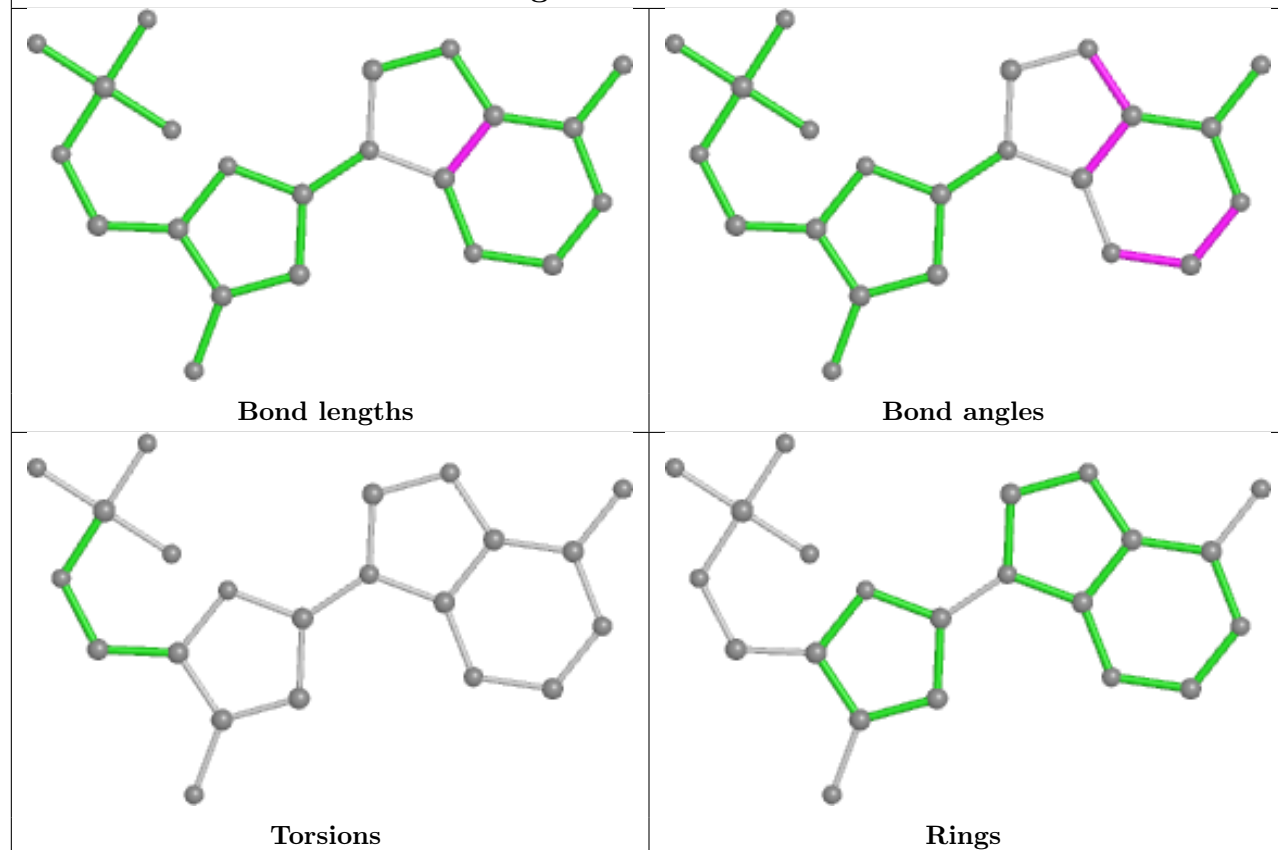


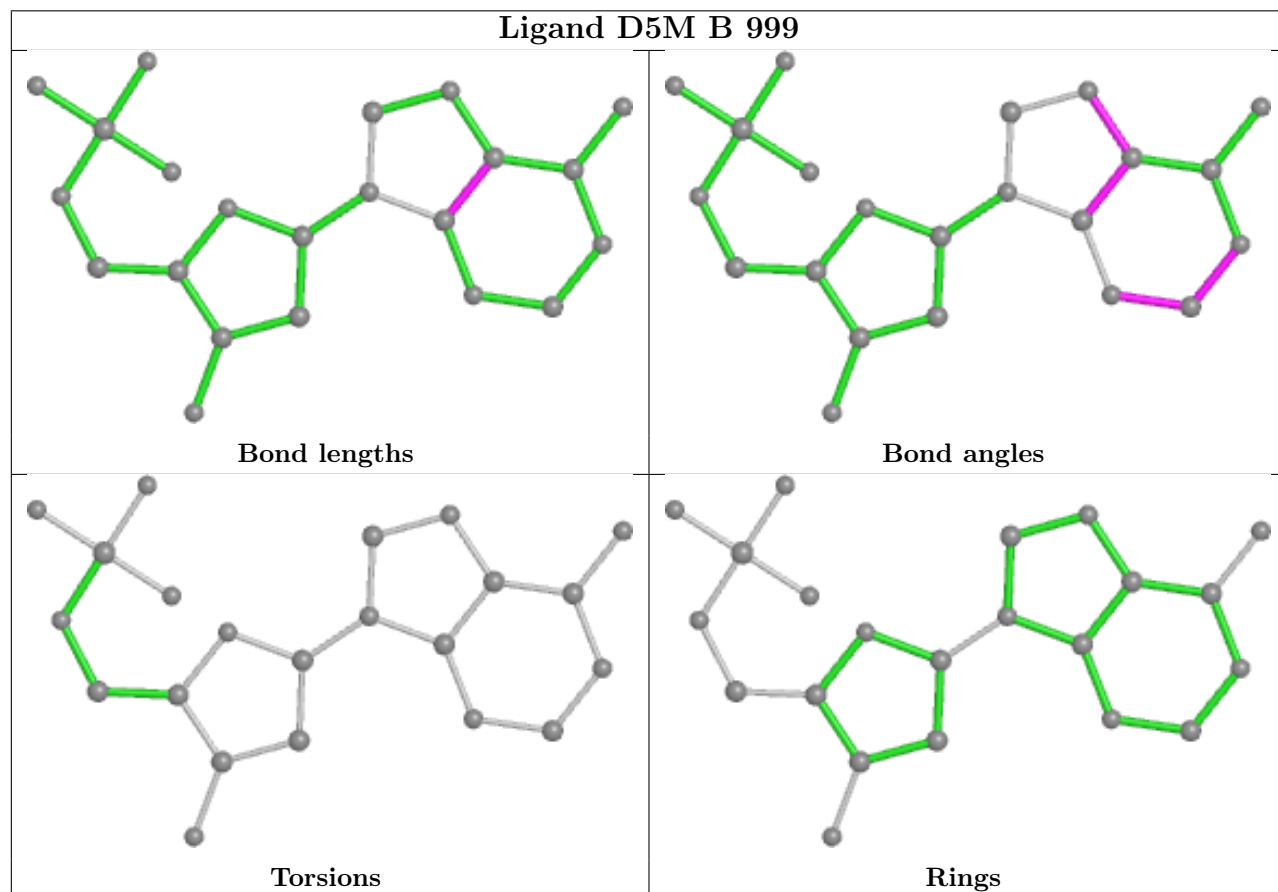
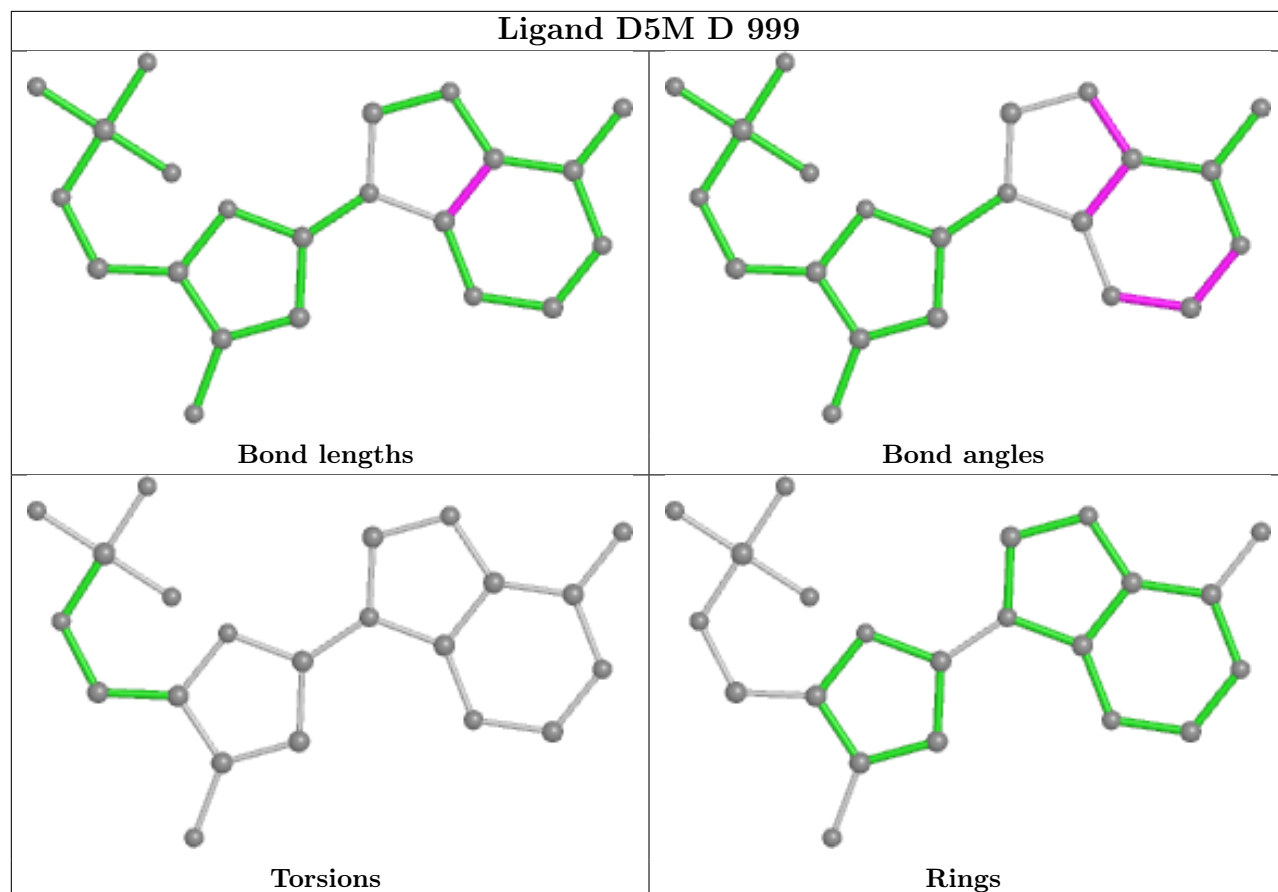


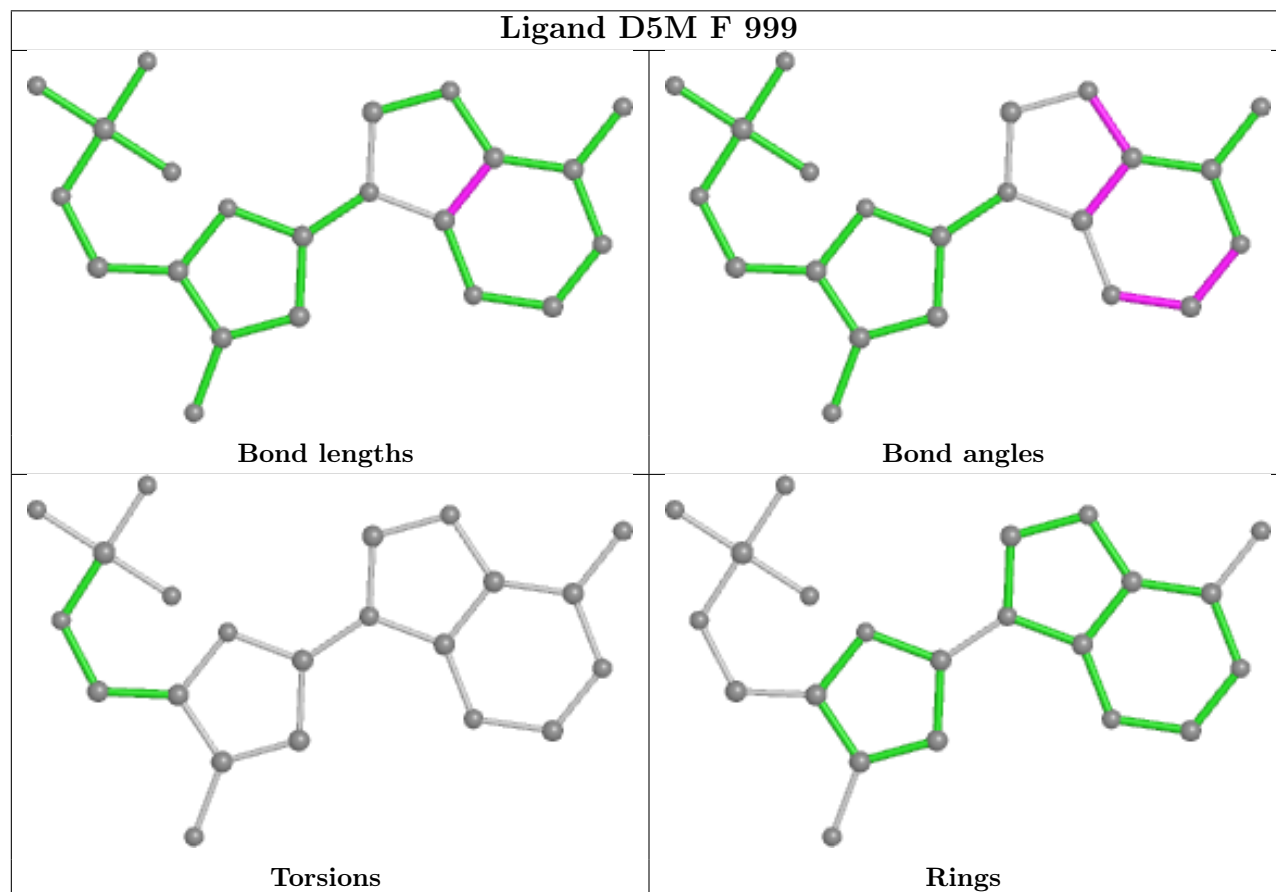
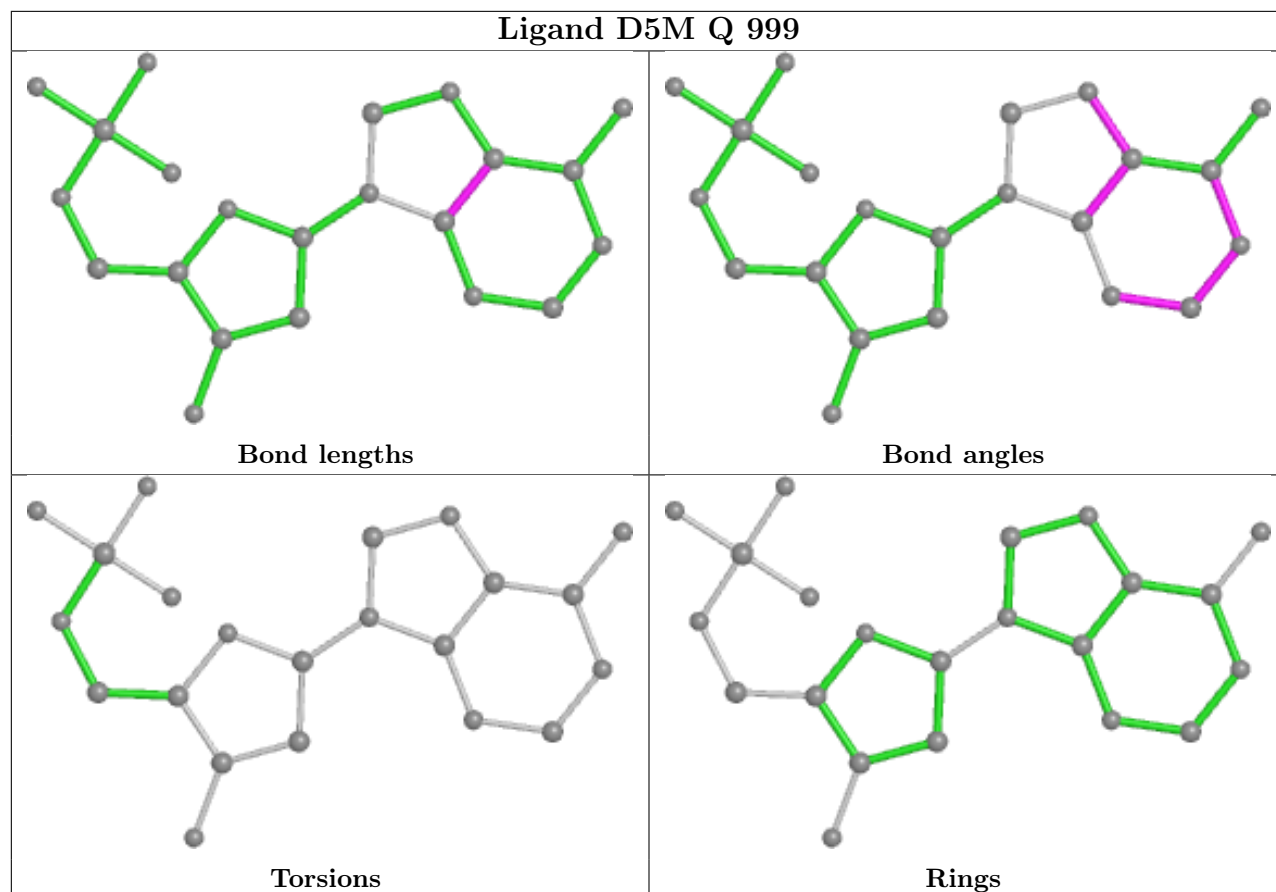
## Ligand D5M S 999



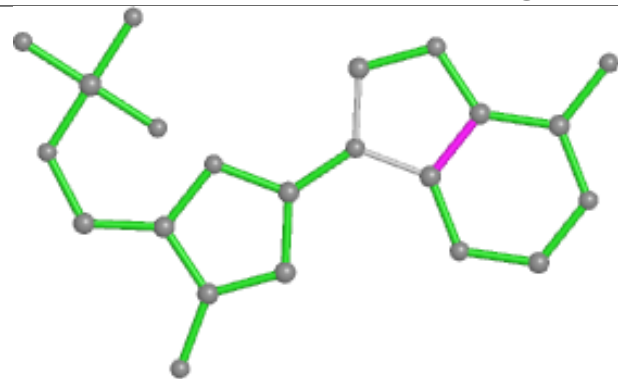
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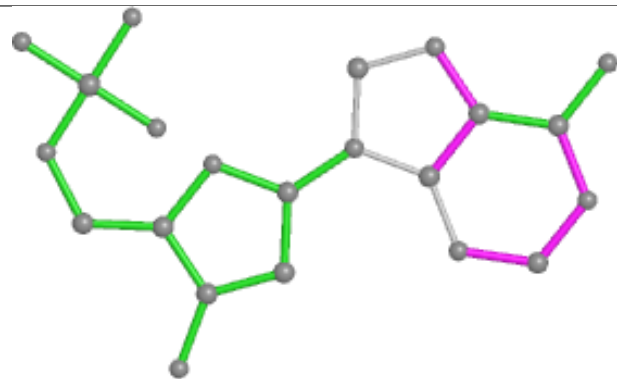




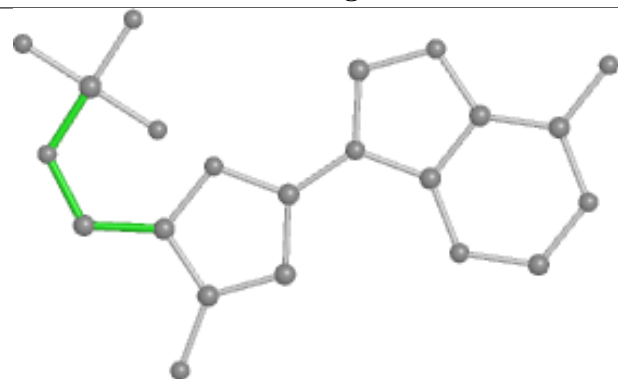
## Ligand D5M L 999



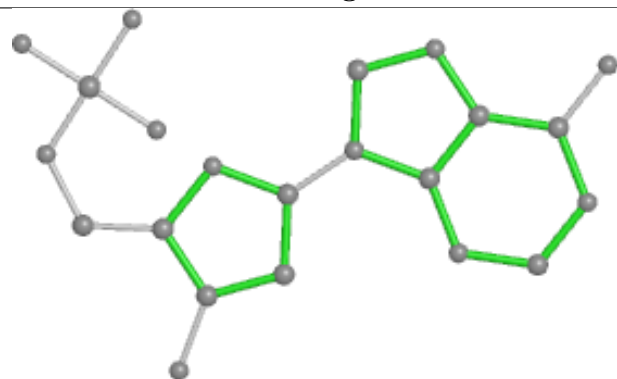
Bond lengths



Bond angles

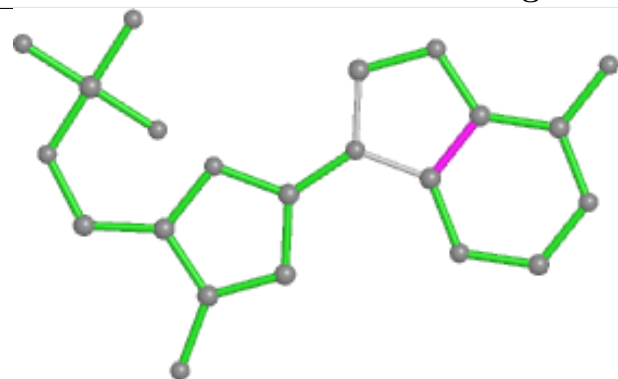


Torsions

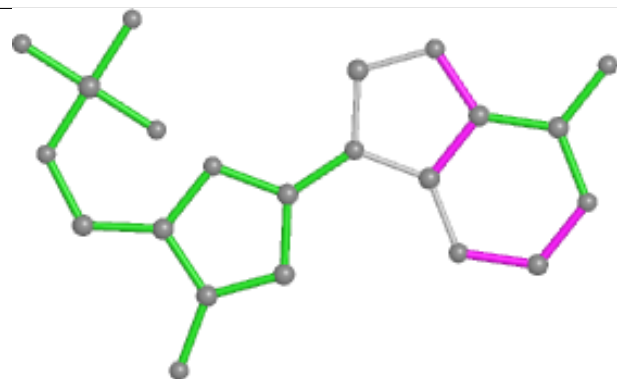


Rings

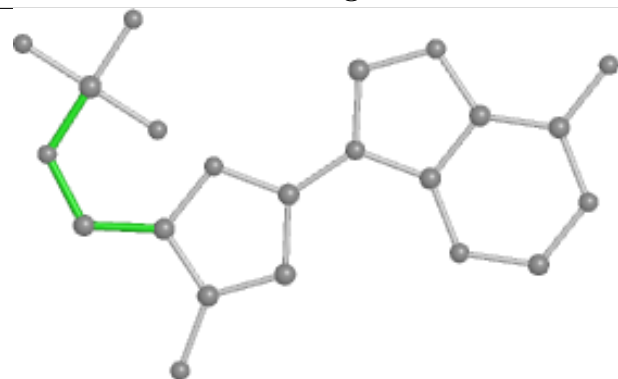
## Ligand D5M I 999



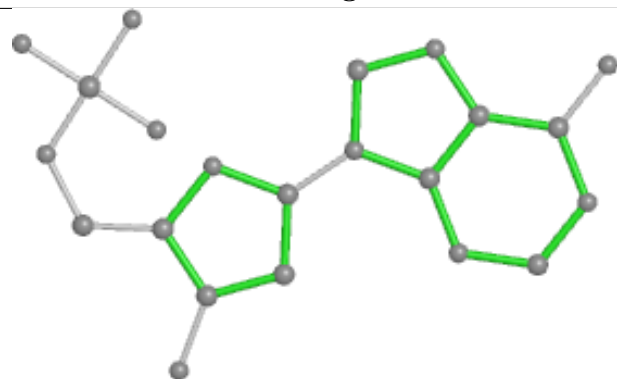
Bond lengths



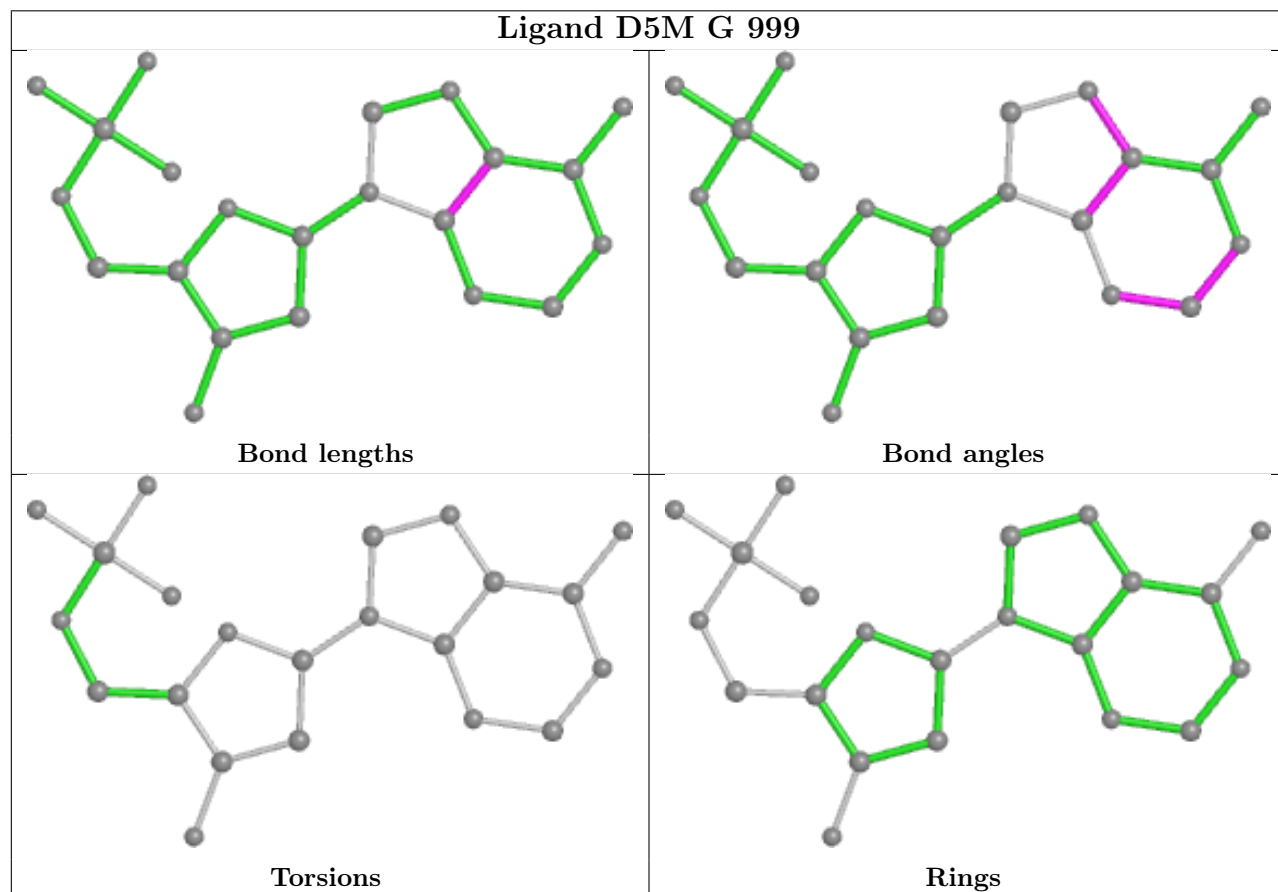
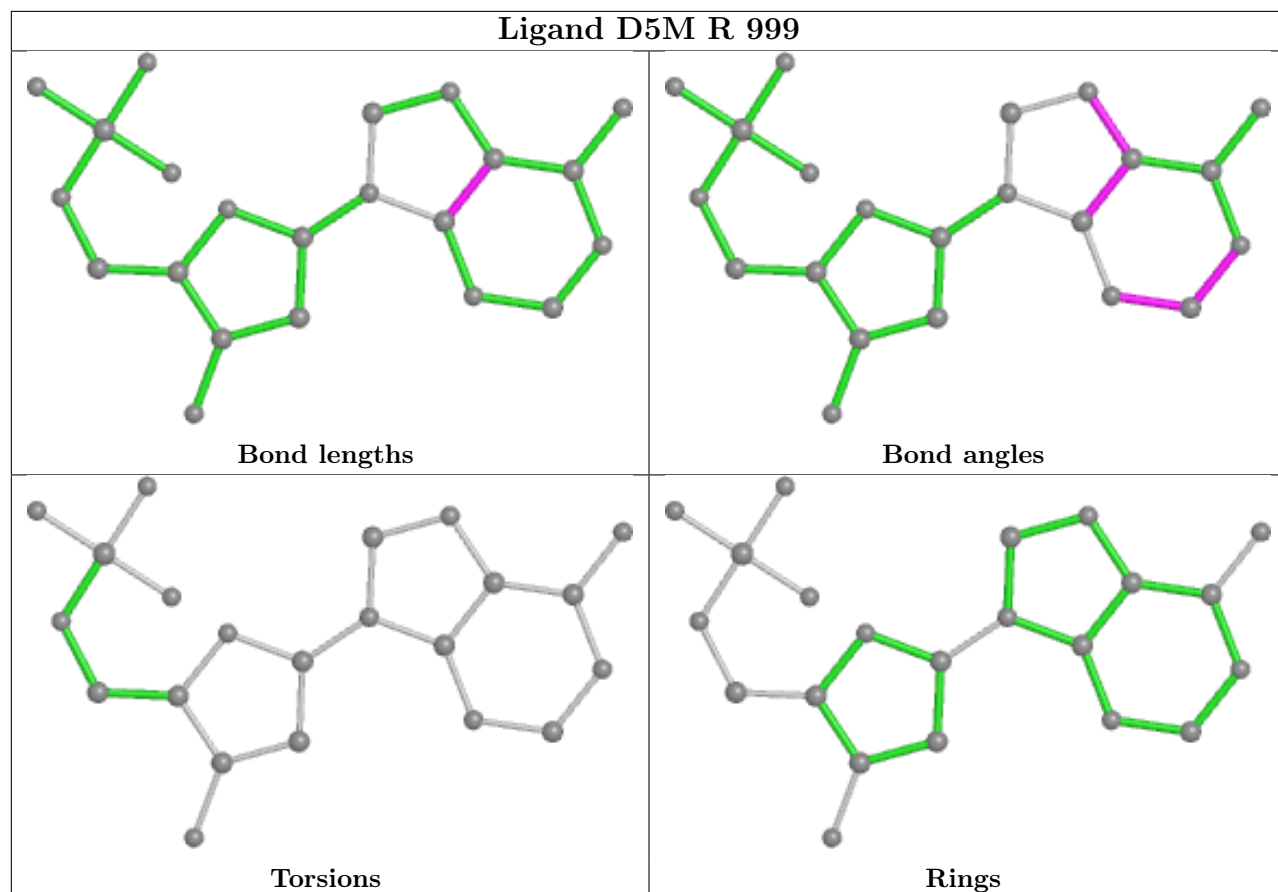
Bond angles



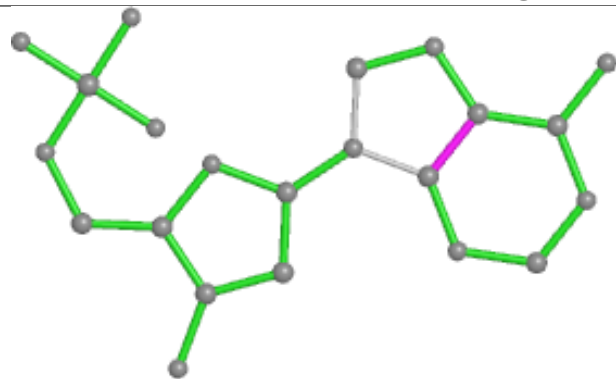
Torsions



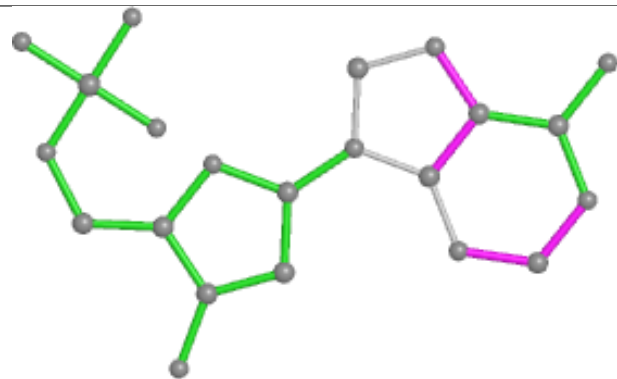
Rings



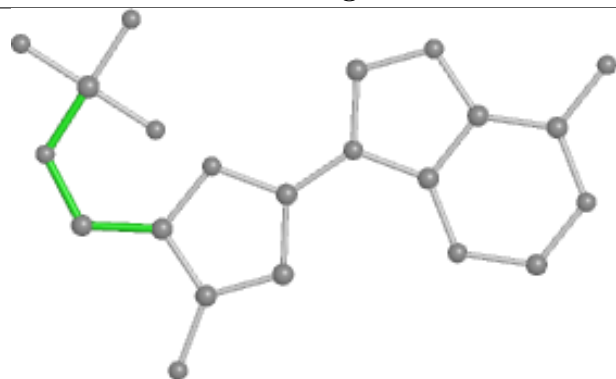
## Ligand D5M E 999



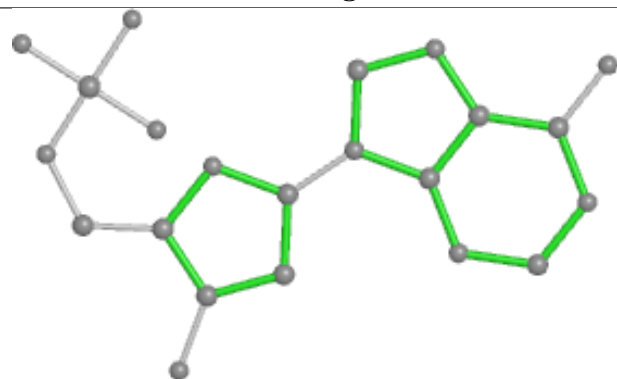
Bond lengths



Bond angles

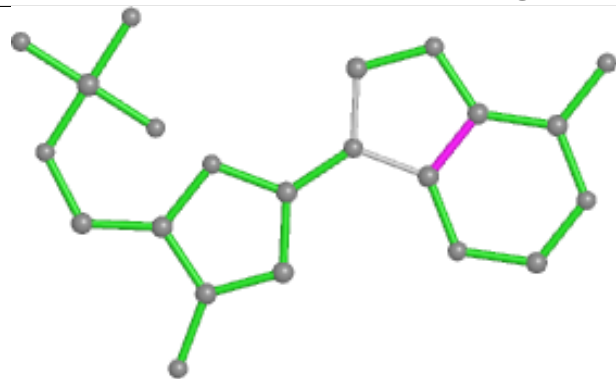


Torsions

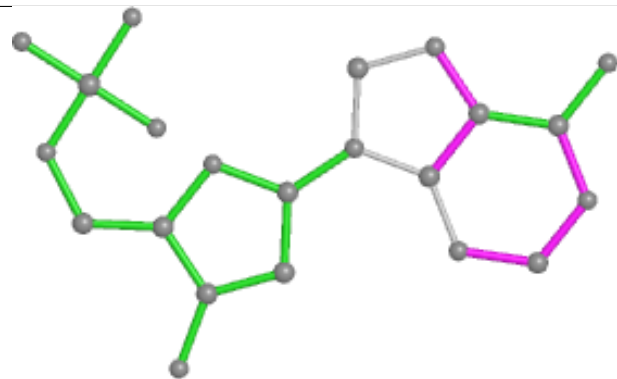


Rings

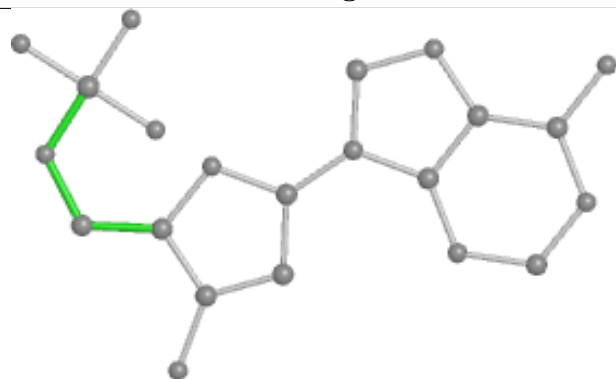
## Ligand D5M C 999



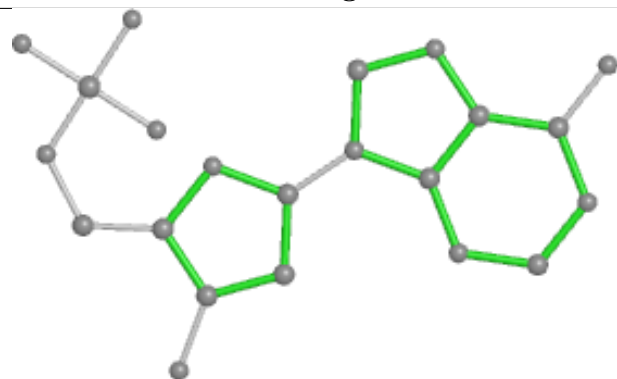
Bond lengths



Bond angles

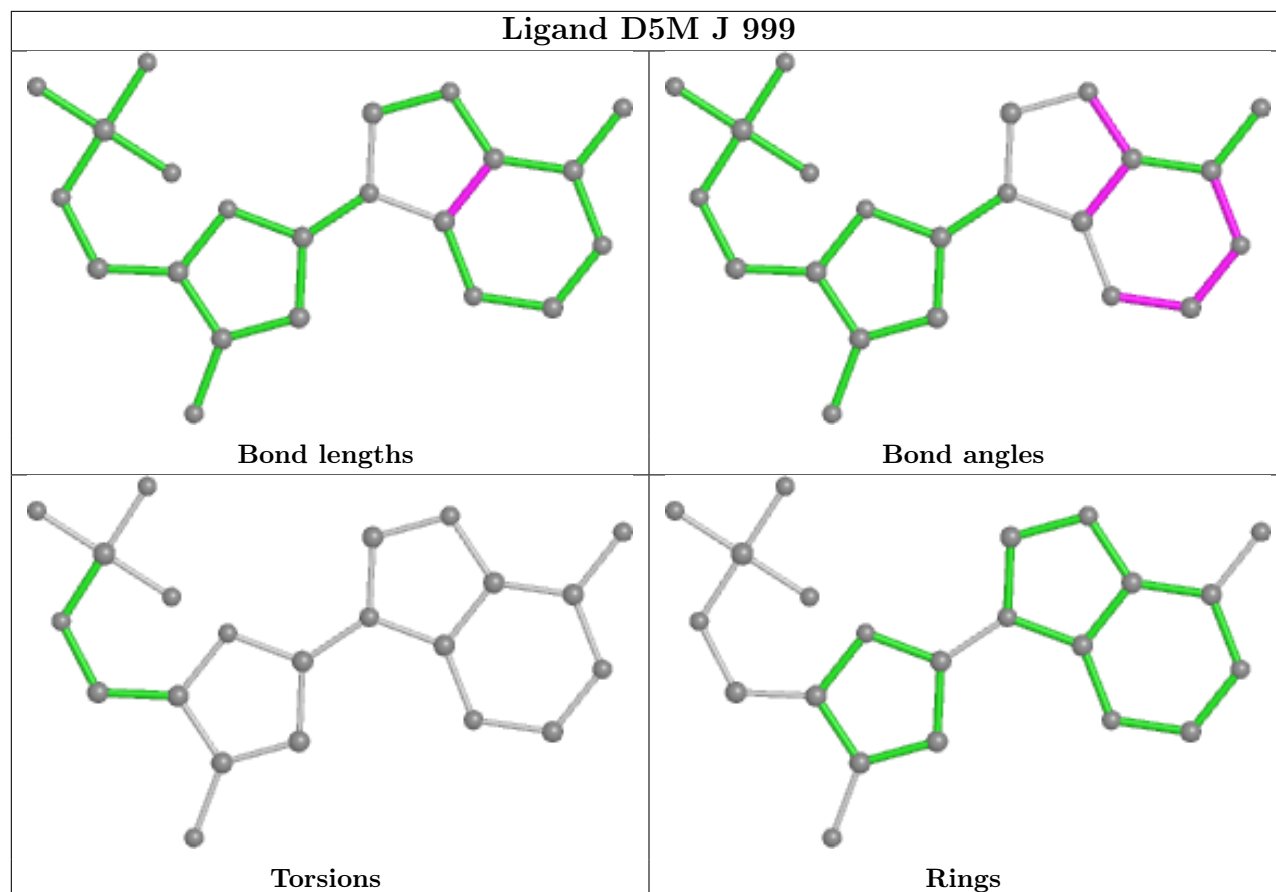


Torsions

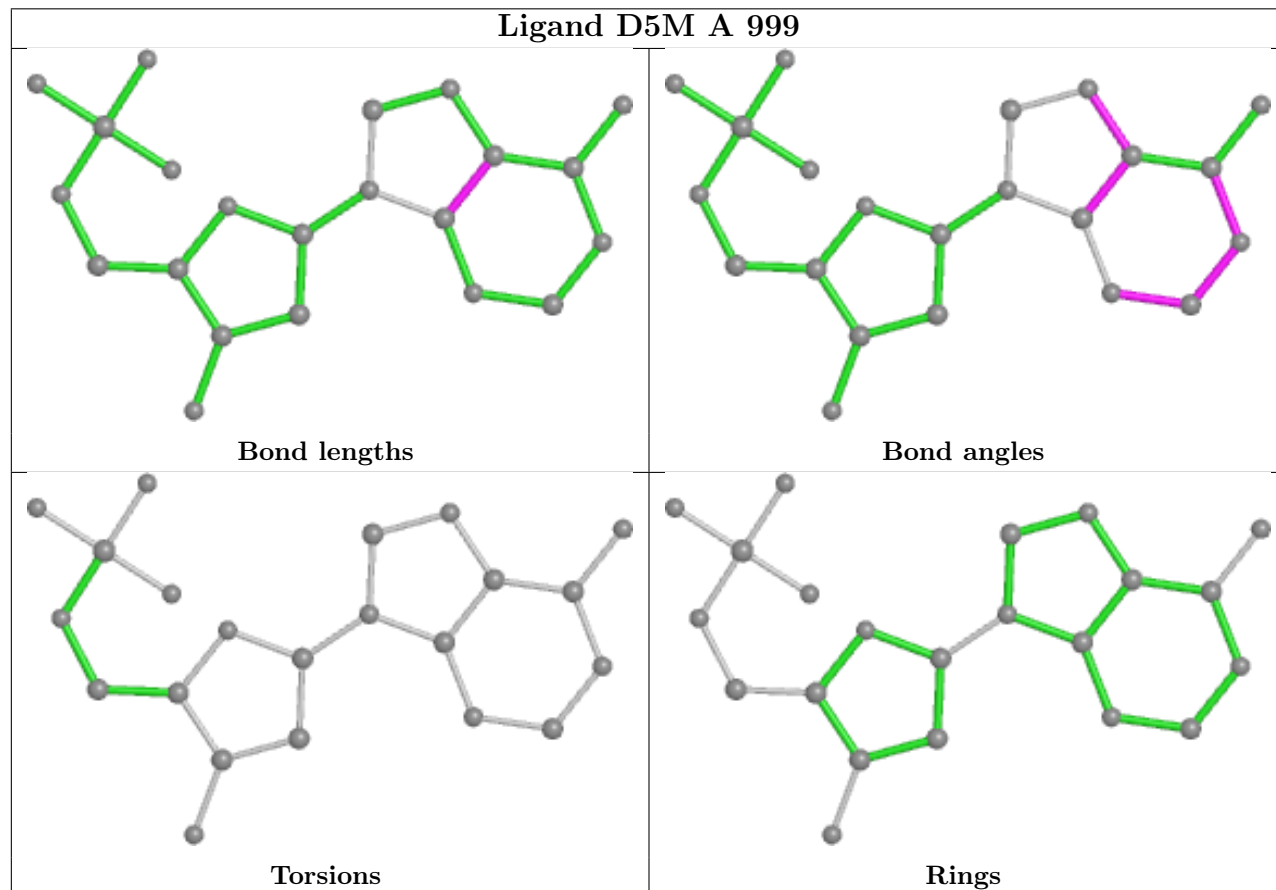


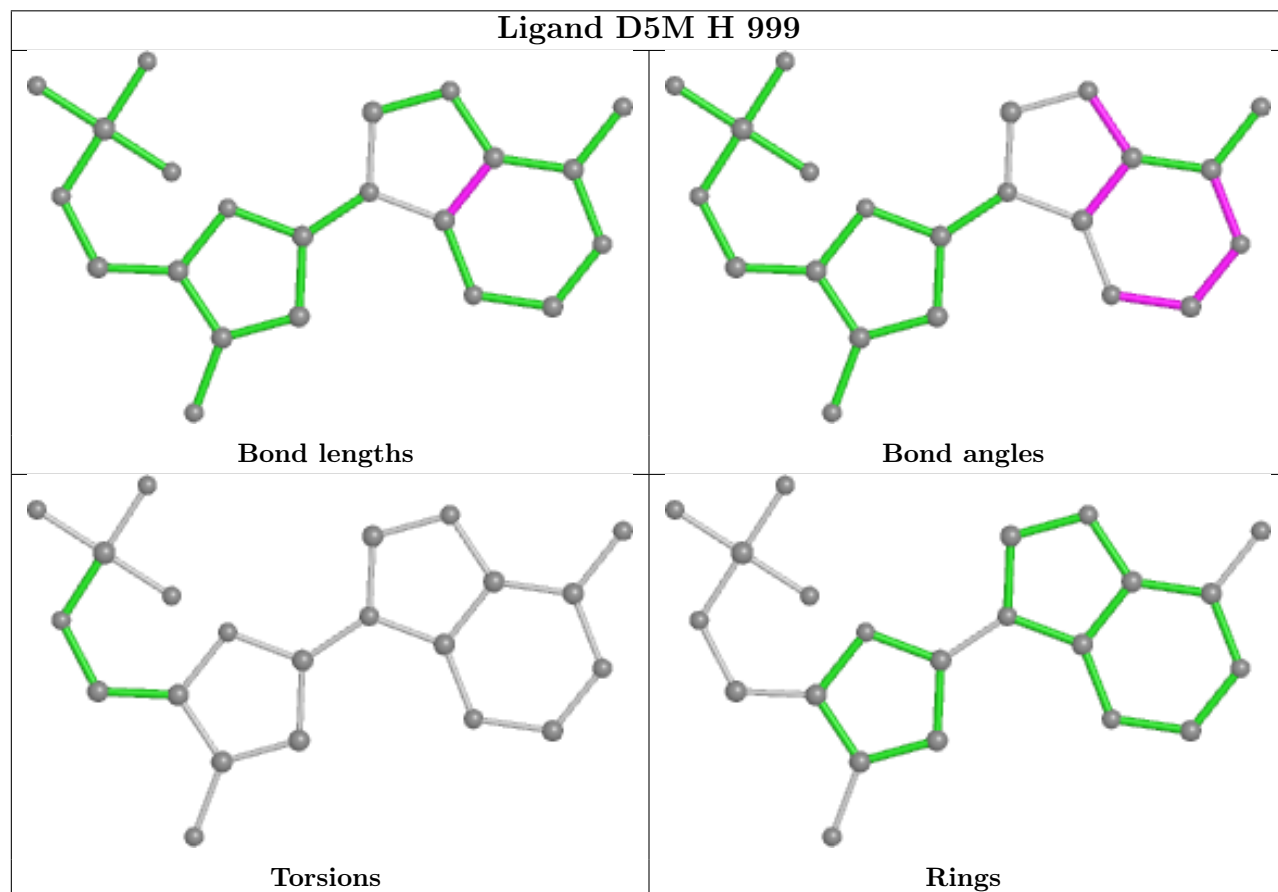
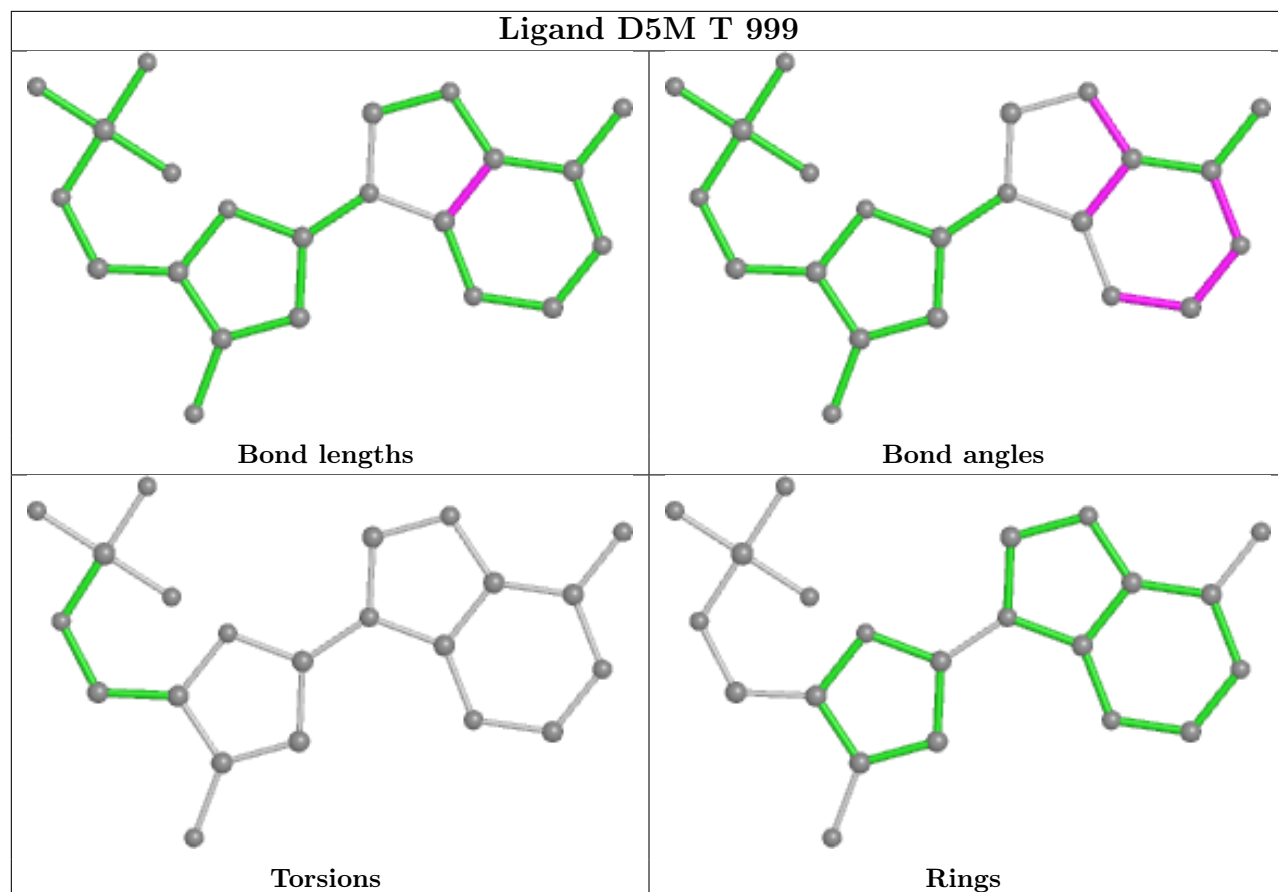
Rings

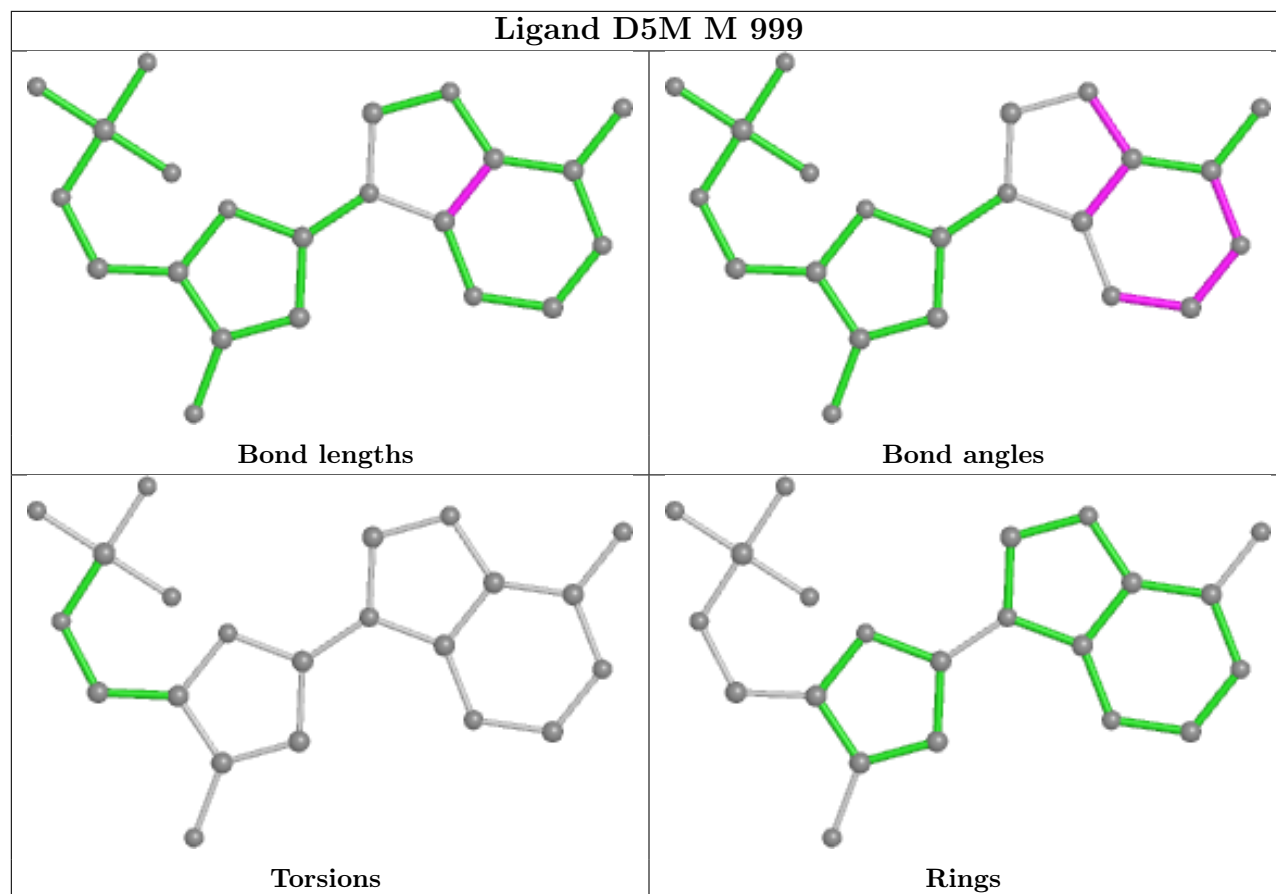
## Ligand D5M J 999



## Ligand D5M A 999







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	520/736 (70%)	-0.07	3 (0%) 89 88	65, 88, 125, 152	0
1	B	520/736 (70%)	-0.09	5 (0%) 82 80	65, 88, 125, 152	0
1	C	520/736 (70%)	-0.10	5 (0%) 82 80	65, 88, 125, 152	0
1	D	520/736 (70%)	-0.07	4 (0%) 86 84	65, 88, 125, 152	0
1	E	520/736 (70%)	-0.05	4 (0%) 86 84	65, 88, 125, 152	0
1	F	520/736 (70%)	-0.05	4 (0%) 86 84	65, 88, 125, 152	0
1	G	520/736 (70%)	-0.00	2 (0%) 92 91	65, 88, 125, 152	0
1	H	520/736 (70%)	-0.05	4 (0%) 86 84	65, 88, 125, 152	0
1	I	520/736 (70%)	-0.04	5 (0%) 82 80	65, 88, 125, 152	0
1	J	520/736 (70%)	-0.13	3 (0%) 89 88	65, 88, 125, 152	0
1	K	520/736 (70%)	-0.01	3 (0%) 89 88	65, 88, 125, 152	0
1	L	520/736 (70%)	-0.10	4 (0%) 86 84	65, 88, 125, 152	0
1	M	520/736 (70%)	-0.13	5 (0%) 82 80	65, 88, 125, 152	0
1	N	520/736 (70%)	-0.14	2 (0%) 92 91	65, 88, 125, 152	0
1	O	520/736 (70%)	-0.10	1 (0%) 95 95	65, 88, 125, 152	0
1	P	520/736 (70%)	-0.07	3 (0%) 89 88	65, 88, 125, 152	0
1	Q	520/736 (70%)	-0.02	3 (0%) 89 88	65, 88, 125, 152	0
1	R	520/736 (70%)	-0.06	6 (1%) 79 76	65, 88, 125, 152	0
1	S	520/736 (70%)	-0.07	2 (0%) 92 91	65, 88, 125, 152	0
1	T	520/736 (70%)	-0.08	3 (0%) 89 88	65, 88, 125, 152	0
All	All	10400/14720 (70%)	-0.07	71 (0%) 87 86	65, 88, 125, 152	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	GLY	5.0
1	N	217	GLY	4.9
1	Q	217	GLY	4.7
1	R	218	ALA	4.6
1	I	217	GLY	4.4

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

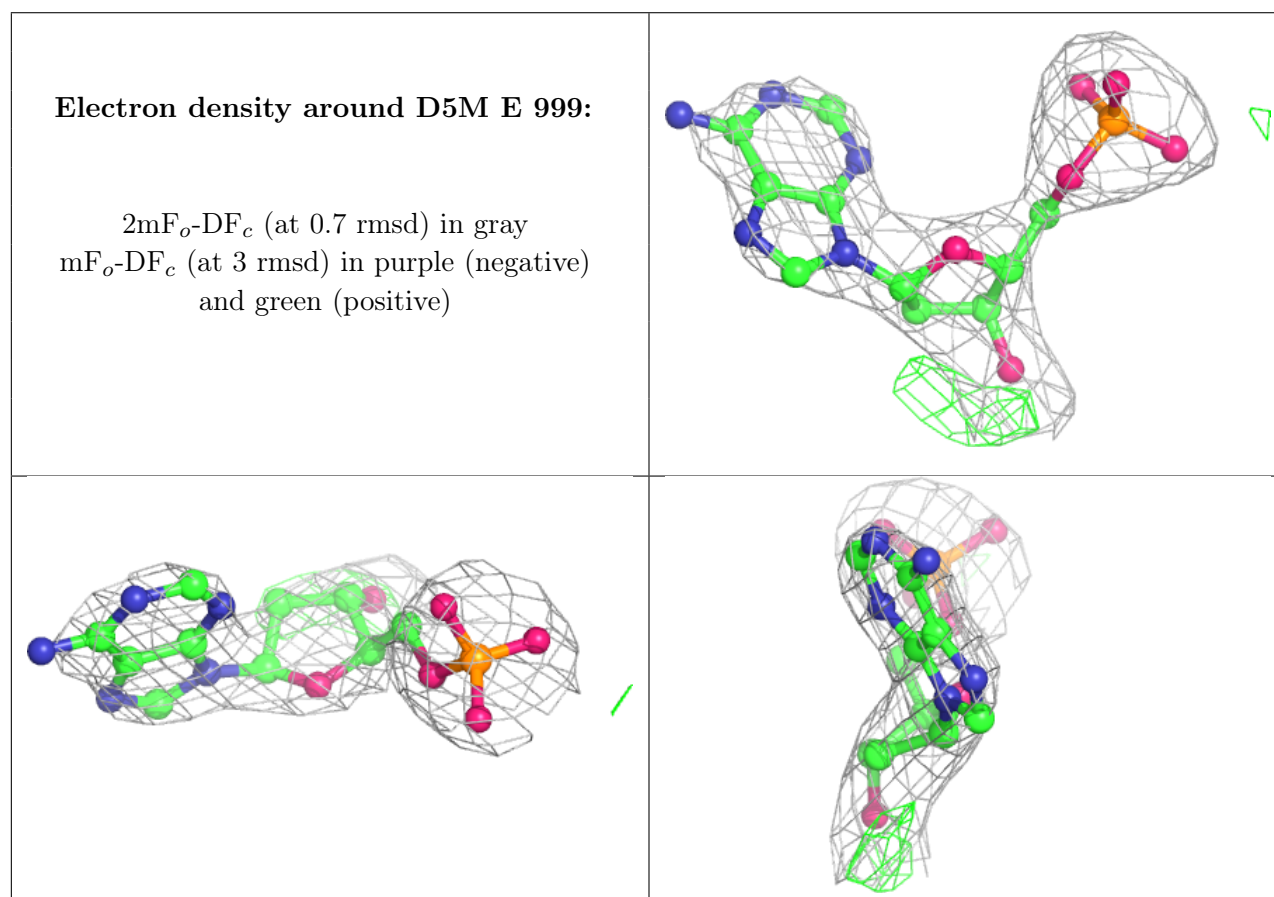
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	D5M	E	999	22/22	0.87	0.30	81,81,81,81	22
2	D5M	N	999	22/22	0.90	0.28	81,81,81,81	22
2	D5M	D	999	22/22	0.91	0.23	81,81,81,81	22
2	D5M	K	999	22/22	0.92	0.19	81,81,81,81	22
2	D5M	P	999	22/22	0.92	0.19	81,81,81,81	22
2	D5M	T	999	22/22	0.92	0.30	81,81,81,81	22
2	D5M	I	999	22/22	0.93	0.23	81,81,81,81	22
2	D5M	B	999	22/22	0.93	0.25	81,81,81,81	22
2	D5M	M	999	22/22	0.93	0.31	81,81,81,81	22
2	D5M	F	999	22/22	0.93	0.26	81,81,81,81	22
2	D5M	G	999	22/22	0.93	0.23	81,81,81,81	22
2	D5M	R	999	22/22	0.93	0.25	81,81,81,81	22
2	D5M	S	999	22/22	0.93	0.22	81,81,81,81	22
2	D5M	H	999	22/22	0.93	0.25	81,81,81,81	22
2	D5M	O	999	22/22	0.94	0.26	81,81,81,81	22
2	D5M	A	999	22/22	0.94	0.23	81,81,81,81	22
2	D5M	Q	999	22/22	0.94	0.22	81,81,81,81	22
2	D5M	L	999	22/22	0.94	0.27	81,81,81,81	22
2	D5M	C	999	22/22	0.94	0.22	81,81,81,81	22

*Continued on next page...*

*Continued from previous page...*

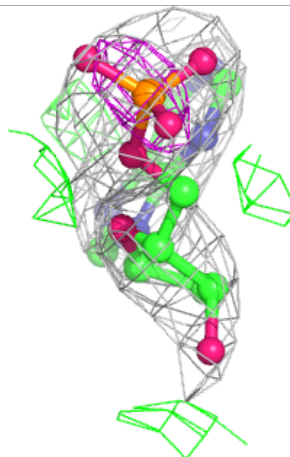
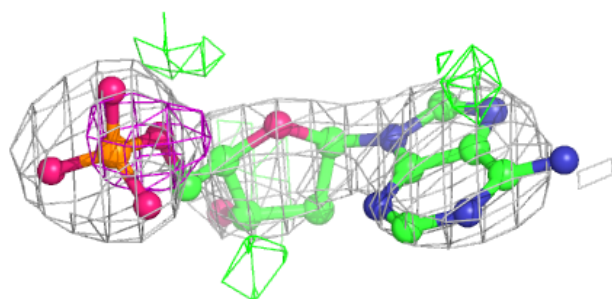
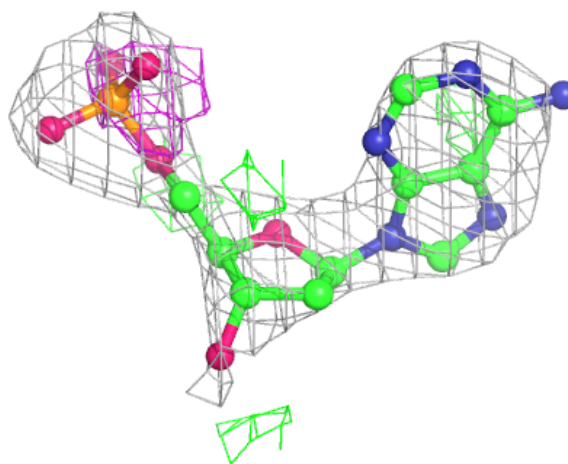
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	D5M	J	999	22/22	0.94	0.19	81,81,81,81	22

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



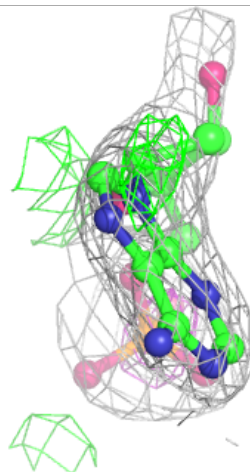
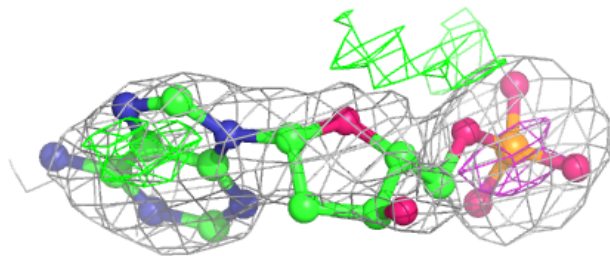
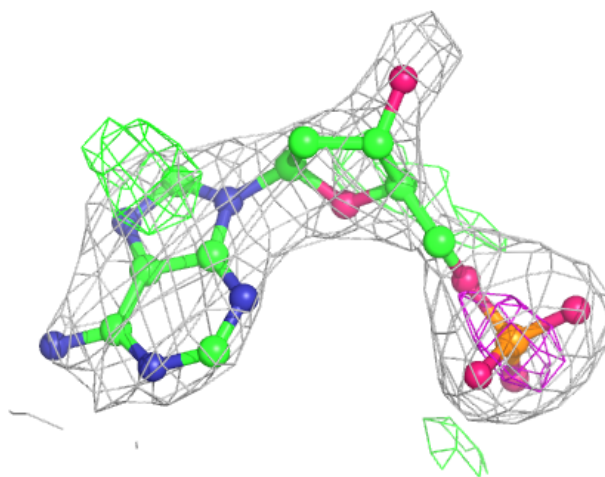
**Electron density around D5M N 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



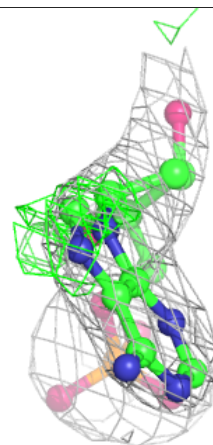
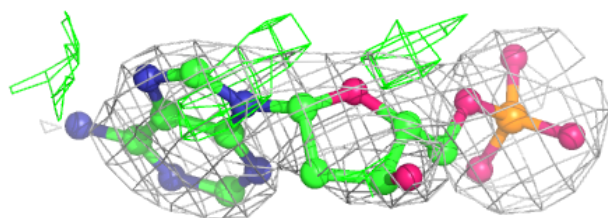
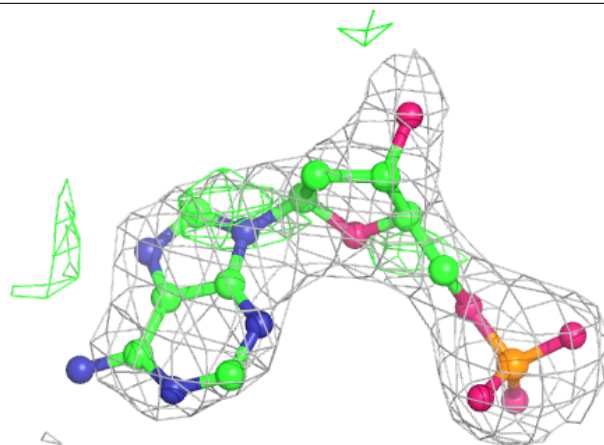
**Electron density around D5M D 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



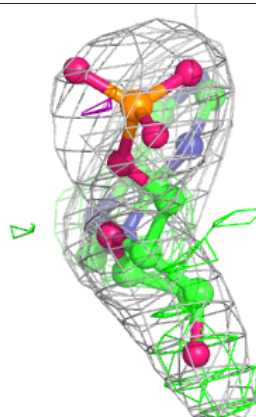
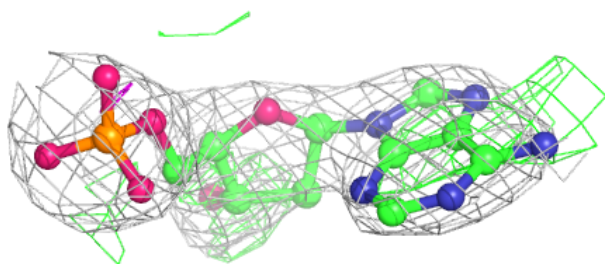
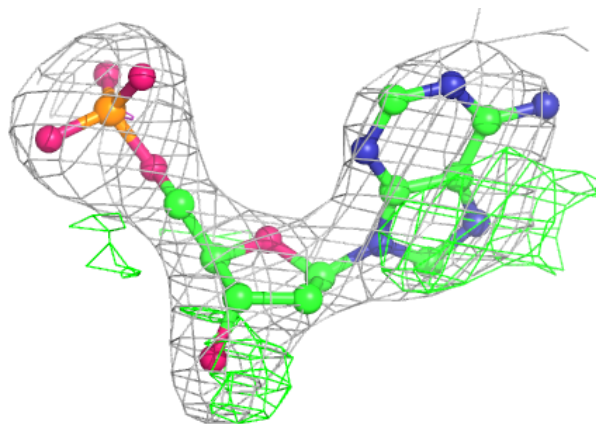
**Electron density around D5M K 999:**

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and green (positive)

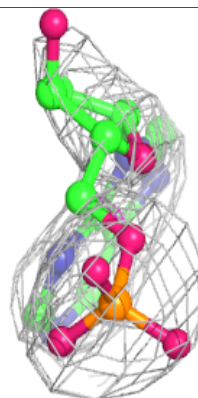
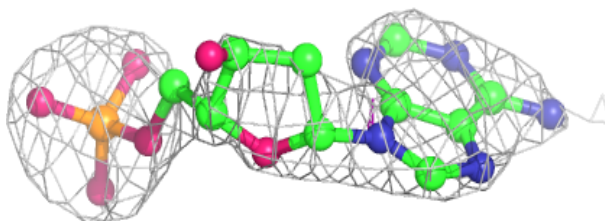
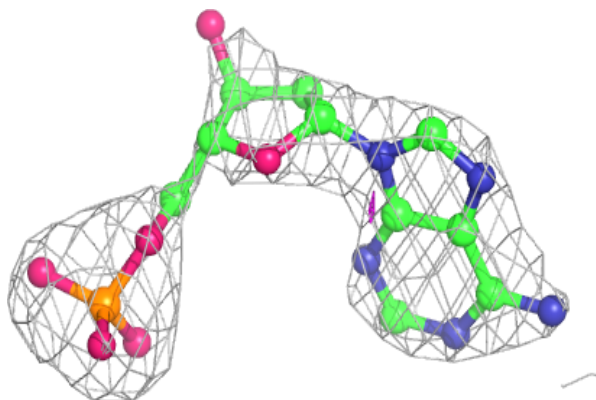


**Electron density around D5M P 999:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

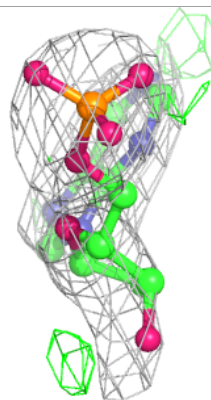
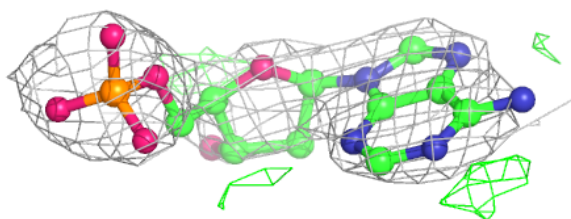
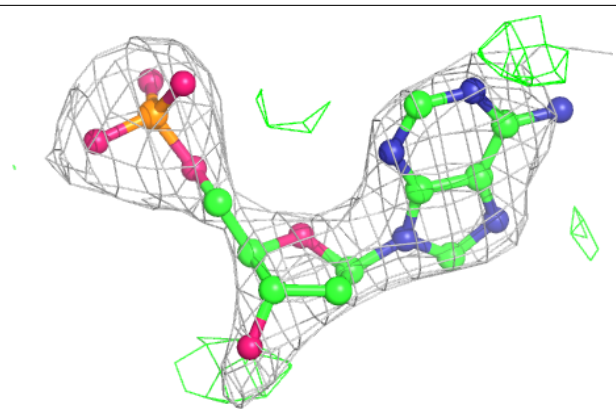
**Electron density around D5M T 999:**

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and green (positive)



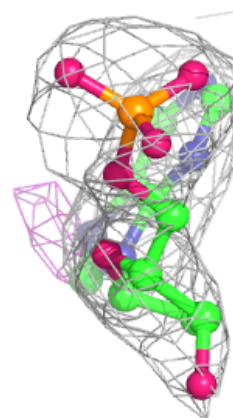
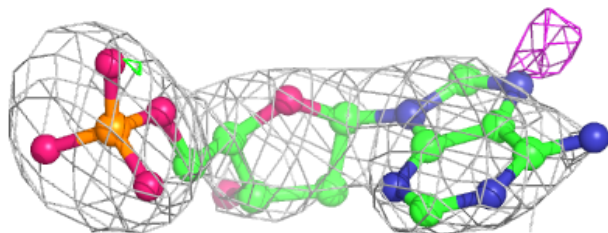
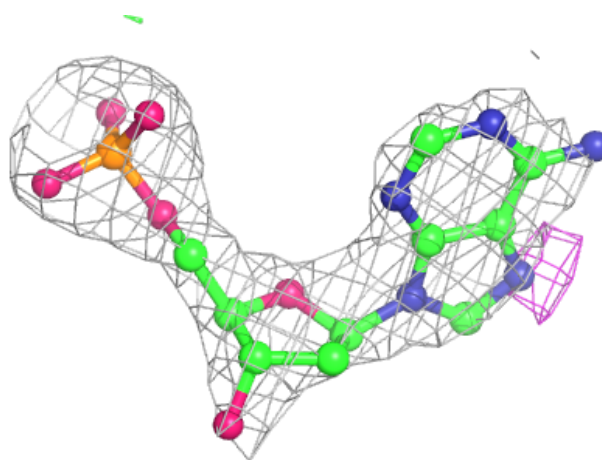
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and green (positive)



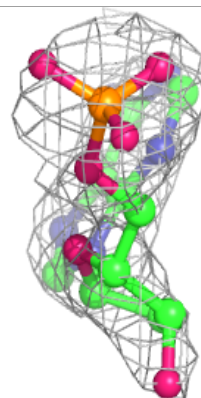
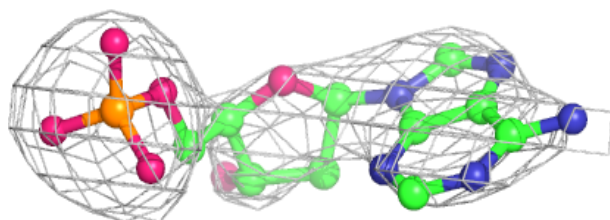
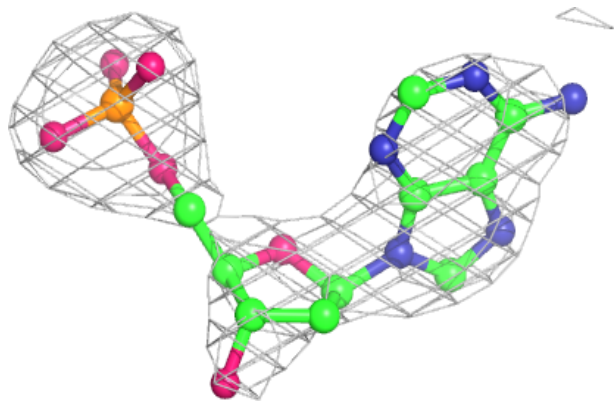
**Electron density around D5M B 999:**

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and green (positive)

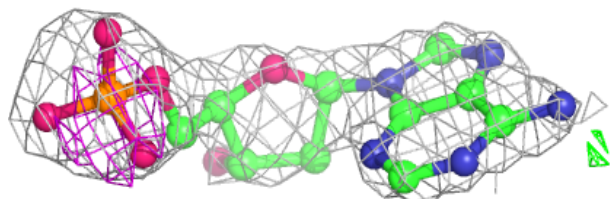
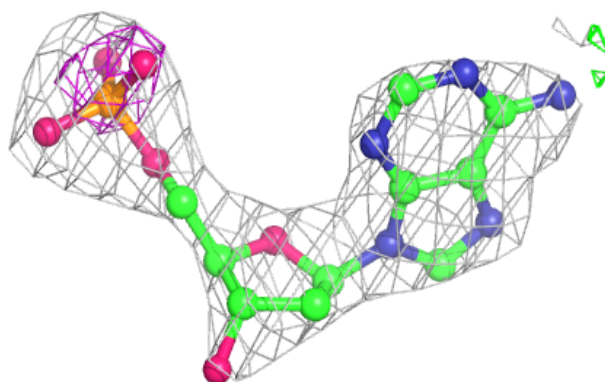


**Electron density around D5M M 999:**

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and green (positive)

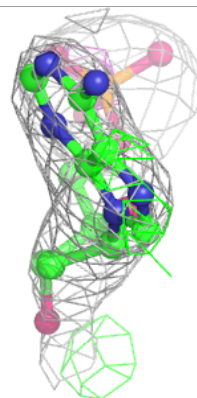
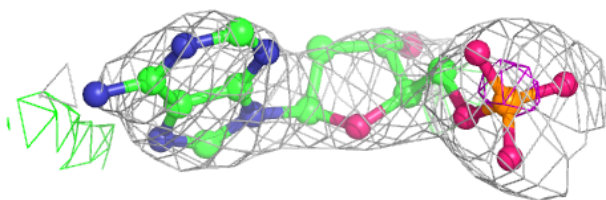
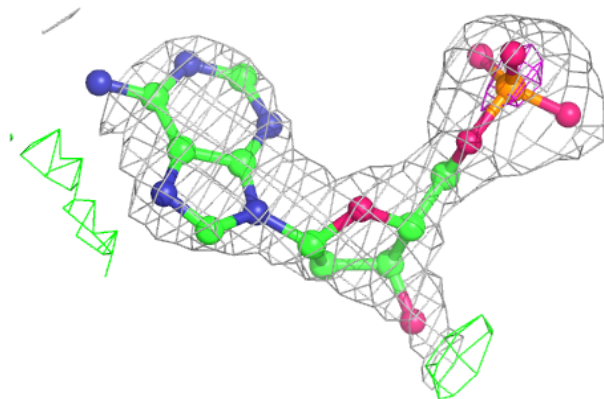
**Electron density around D5M F 999:**

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and green (positive)

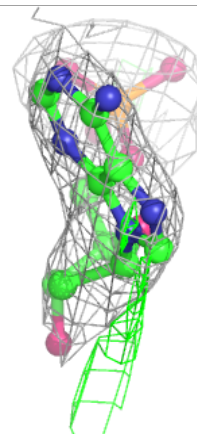
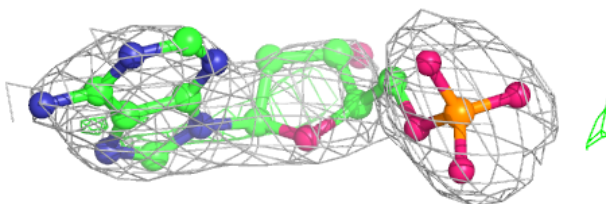
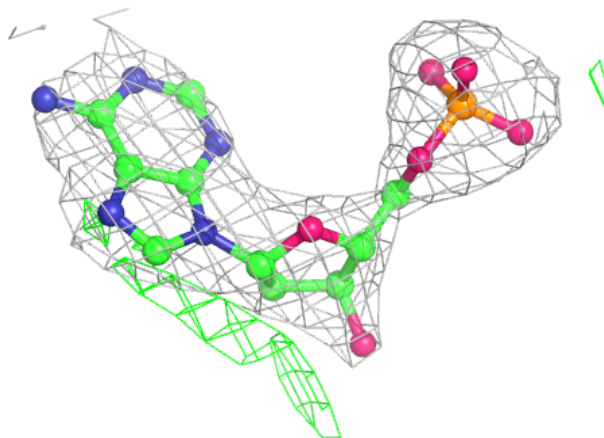


**Electron density around D5M G 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

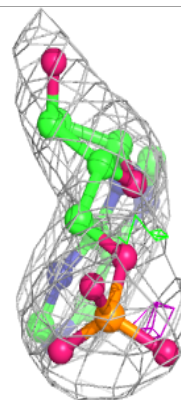
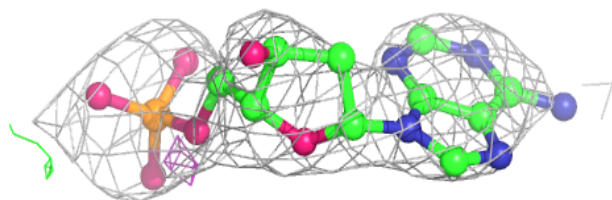
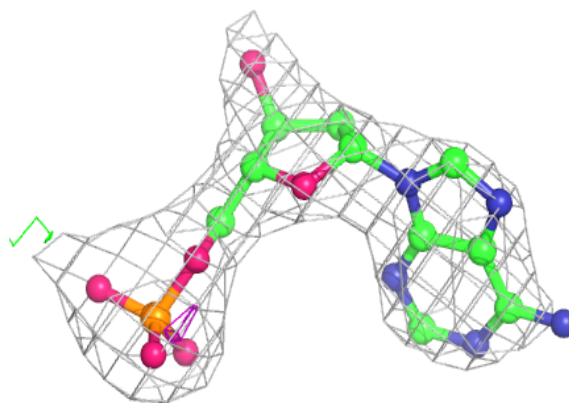
**Electron density around D5M R 999:**

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and green (positive)

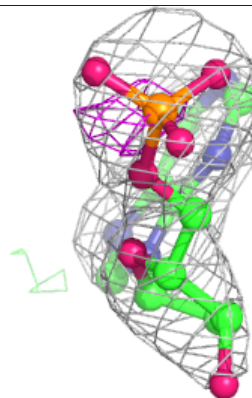
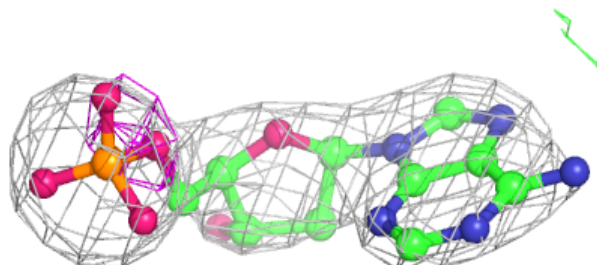
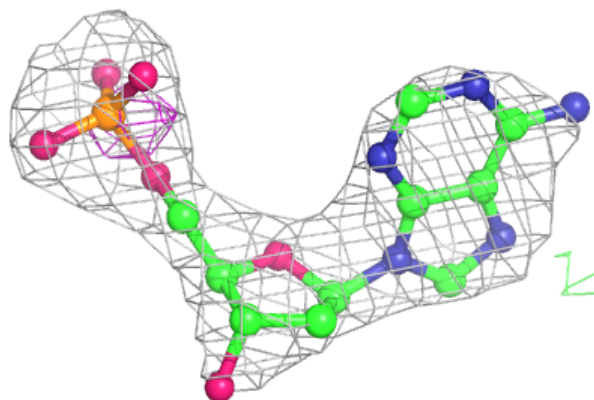


**Electron density around D5M S 999:**

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and green (positive)

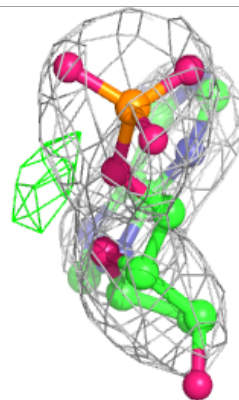
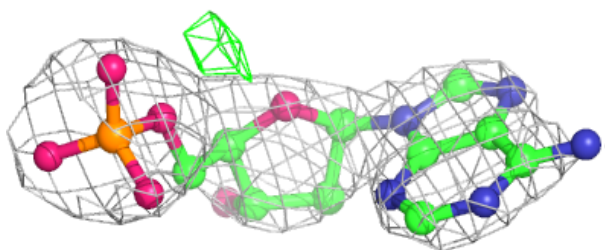
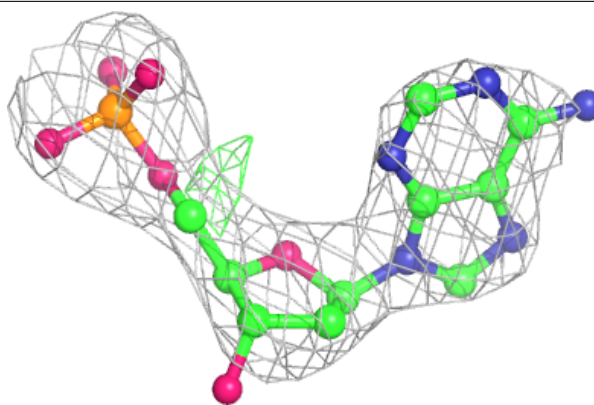
**Electron density around D5M H 999:**

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and green (positive)

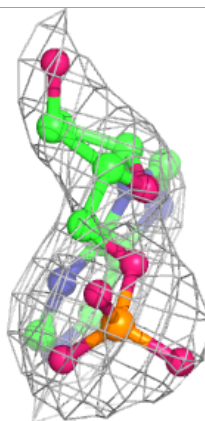
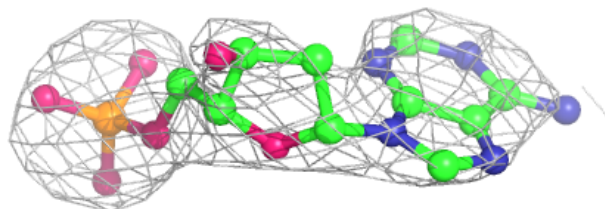
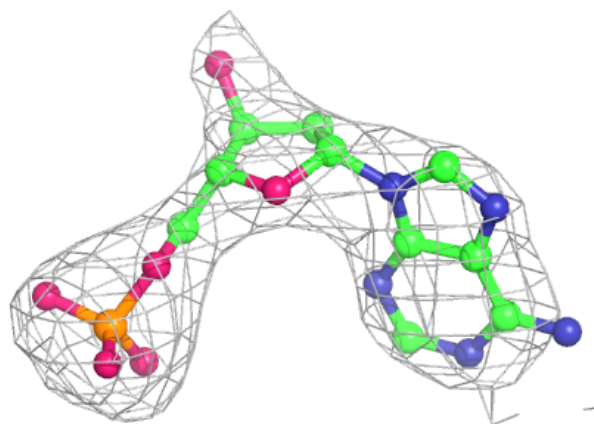


**Electron density around D5M O 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

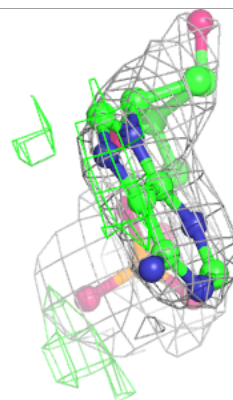
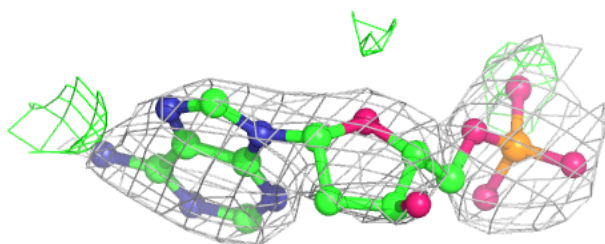
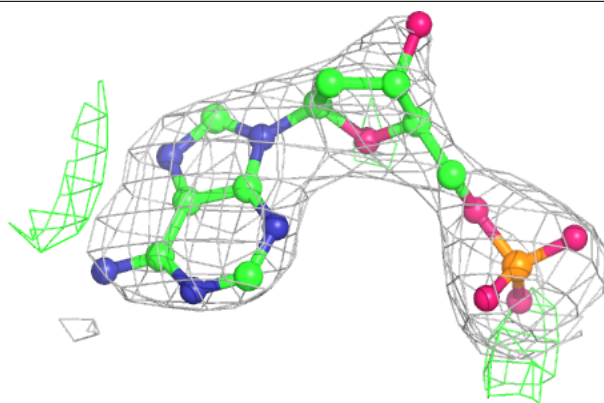
**Electron density around D5M A 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

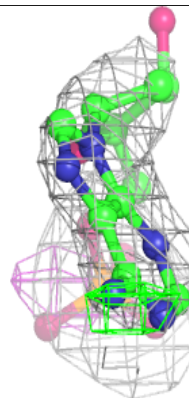
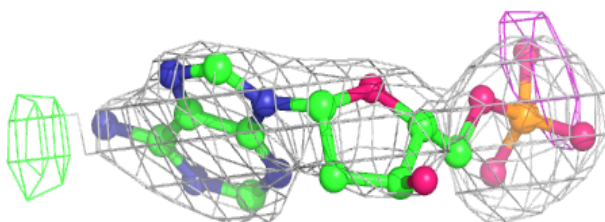
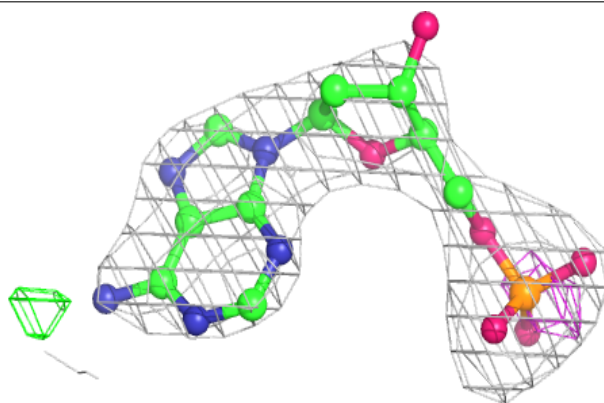


**Electron density around D5M Q 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

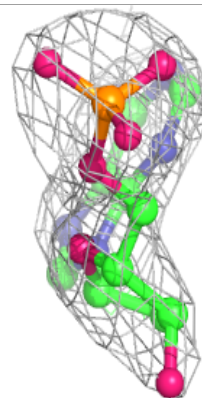
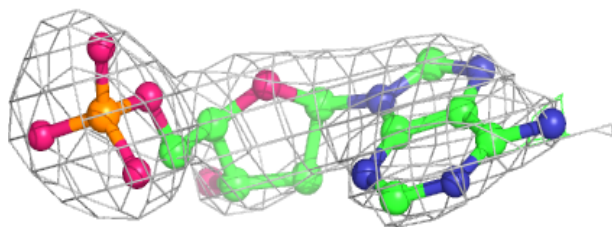
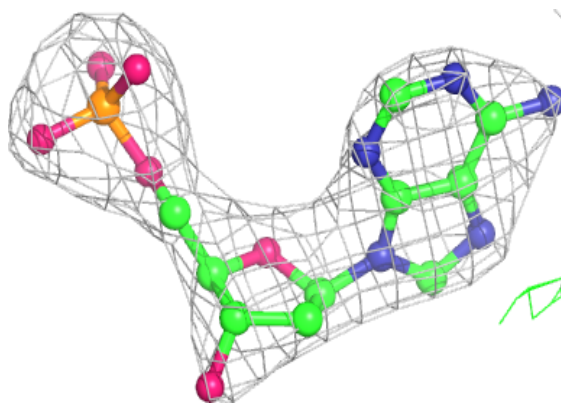
**Electron density around D5M L 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

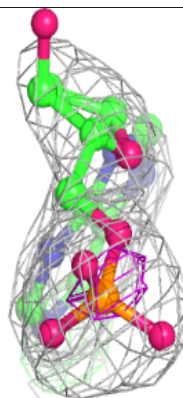
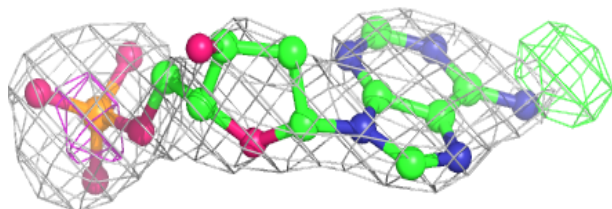
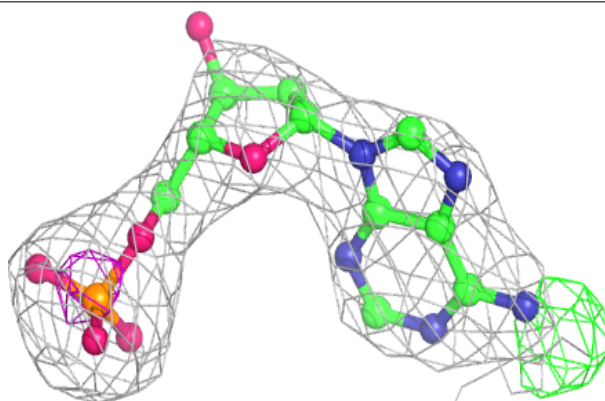


**Electron density around D5M C 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around D5M J 999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.